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FEATURING

Dr. Mark Freeman

Inspiring Change through Curiosity and Innovation

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Eureka is a student-founded and student-run initiative. This journal offers undergraduate scientists the unique opportunity to share their discoveries with the scientific world through the peer review process. *Eureka* is an educational institution, with a diverse team of reviewers from many scientific backgrounds, exposing undergraduate students to the publication process often excluded from their traditional scientific education. Through clear and effective scientific writing, students will be able to work together with faculty members to contribute original research and promote science.

Our mission is to support and promote quality, peer-reviewed research by undergraduate scientists across Canada.

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Focused Chaos: An Art in Sciences?

December 2024

Ehsan Misaghi is an MD/PhD student at the University of Alberta. Here, he shares his experience of finding passion through the process of "focused chaos."

Just a few days before I was asked to write this editorial, I attended a webinar during which I found myself rewatching a YouTube video, probably for the 10th time. The video was about the process within the design organization IDEO, which is known for making everything from shoes to toothbrushes to high-tech medical equipment. What's fascinating is how their team, composed of people from vastly different fields, comes together to brainstorm and innovate. At one point, someone describes their process saying, "*It's not organized. What it is, it's focused chaos.*"

The phrase "focused chaos" really resonated with me. Funnily enough, it was my "Invisible Gorilla" moment – the one Christopher Chabris and Daniel Simons implemented in their selective attention test.[1] I had watched the video countless times, but somehow, I had always glossed over this phrase until that day. Once I noticed it, I couldn't let it go. I wrote "focused chaos" on sticky notes and plastered them around my workspace and even on my meal-planning whiteboard (which, let's be honest, hasn't been used for actual meal planning in over a year). Why did it resonate? Because it perfectly captures my journey through science and research, perhaps even my life.

Like many students, I've dabbled in what feels like a thousand different things, and I'm still not entirely sure if I've found the one. But I've come to think of finding one's passion not as a singular, linear pursuit but as a convoluted process that thrives in "focused chaos". There's so much to learn and so many directions to explore. As an undergraduate, I remember constantly hearing about the latest must-know technique, the cutting-edge method that would revolutionize research, or the new field everyone was pivoting toward. Labs are often categorized into neat silos: wet lab, dry lab, basic science, clinical research, but even these boundaries may be easily blurred. And they are! Did you notice AI research getting the Nobel Prize for Physics (and Chemistry)?[2] For someone just starting out, the sheer volume of information can feel overwhelming. So, what should a student, especially an undergraduate, do? My answer is, "*try anything and everything.*"

If something sparks your interest, dive in. Are you passionate about computing science? Find a lab that combines computation with something you care about. Curious about Alzheimer's disease? Work with a team that uses animal models (or cells, or electrical circuits) to unravel its mysteries. Even if these pursuits don't seem connected at first, they might link up later in ways you never expected. And if they don't, you'll still walk away with valuable skills, broader perspectives, and the ability to pull concepts from one field into another. One of the most surprising things I've learned is that research and the generation of new knowledge isn't just about the work; it's also about the people. The relationships you build along the way are just as important as the experiments you run. Some of the most fulfilling moments of my career have come from working alongside brilliant, passionate peers who push me to think differently (or even those who frustrate me at times).

Undergraduate research is, in many ways, the embodiment of focused chaos. It's a mountain of papers to read, experiments to plan, hypotheses to test, and multiple fields to sift through all these again and again. It's the constant tension of balancing coursework, lab work, and, occasionally, the creeping suspicion that you have no idea what you're doing (spoiler: none of us do, at first). But in that chaos, there's also tremendous focus.

When trying new things, mistakes are inevitable. *Being wrong is fine. What isn't fine is failing to learn from those missteps and mishaps.* The fear of failure might be holding us back when trying new things. Worrying about looking unprepared, inexperienced, or even incompetent is easy, especially in an academic setting where excellence often feels like the baseline expectation. I know this is a cliché, but *failure is not the opposite of success; it's a necessary part of it*. And, honestly, it's hard not to learn when you're immersed in research. Research thrives on trial and error, and the most impactful discoveries often come after countless failed attempts. Every failed experiment is a lesson in problem-solving and, let me tell you, that makes you a highly desired and hireable candidate, for almost any job. For researchers, especially as an undergrad, the first step is the hardest: embracing the unknown and giving yourself permission to fail. Remember, each failure brings you closer to understanding what doesn't work, and that knowledge is just as valuable as knowing what does. Sure, you can't publish null results alone, but you can publish them together with other results, or the null result might push you into a different hypothesis that might answer a bigger question. The possibilities are limitless.

My own journey has been anything but straightforward: from a dual degree in engineering to graduate studies in neuroscience to medical school and genetics research. Each step felt, at times, disconnected, and I was asked why I "switched fields." I was always surprised to be asked that question, "but I didn't switch, I didn't pivot, I went with what I liked." Looking back, I see how the pieces fit together, forming a unique combination of experiences that guide my approach to everything in my life today. Life includes work and, as much as I would like to share how I feel about "work-life balance," or what I like to call "work-life synergy," that is for another time (maybe I will be asked to write another editorial again and will write on it then).

I would be remiss if I didn't mention that it's not just the courses and the lab work that matters. Some of my most meaningful learning has come from extracurriculars. Whether it was activism, organizing events, starting new initiatives, or volunteering, these experiences shaped my ability to work with others, manage time, and stay grounded (or sane, at times). If you're wondering whether extracurriculars are worth it; absolutely, they are.

I want to end on the note that our undergraduate and even graduate years are formative. They are a time to explore widely before you "settle" or decide never to settle at all. This is the heart of "focused chaos," and why I love this phrase so much. I have been obsessed with it lately: finding clarity in the mess, purpose in the process, and growth in the challenges. So, to the undergraduate researchers reading this, "embrace the chaos; dive into the things that excite you; don't be afraid to be wrong, to shift directions, or to try something completely new." Whether or not you ever feel like
you've "found your thing," you'll gain skills, relationships, and a perspective that will serve you in whatever comes next. And who knows? One day, you might look back on your own sticky notes, scribbled protocols, or meal-planning whiteboards and realize that in the chaos, you found focus.

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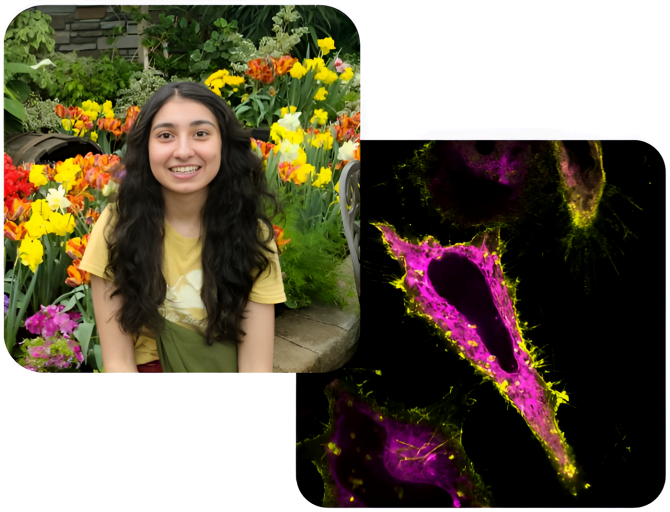
[1] "Invisible Gorilla" is a reference to the selective attention test designed by Chabris and Simons, where participants would miss an appearance of an individual in a gorilla costume in a video, while concentrating on the number of times a ball was passed between players. The experiment illustrates how intense focus on a task can render individuals oblivious to unexpected yet salient events outside their attention.

[2] In 2024, the Nobel prize was awarded for discoveries in computational design of neural networks in Physics, and in protein structure prediction with the use of an AI model in Chemistry.

Ehlam Iftikhar is an undergraduate student in the Faculty of Science. In her physiology program, she is researching sphingomyelinases' role in extracellular vesicle production in Parkinson's disease under her supervisors, Dr. Julie Jacquemyn and Dr. Maria S. Ioannou. Her image titled *Sphingomyelinase: The Hidden Trigger of Parkinson's Progression* is featured on the front cover of the issue.



"While it's important to choose a research topic that excites you, I believe the most crucial factor is finding the right team to work with."

What can you tell us about your research image?

Sphingomyelinases (SMase) are enzymes involved in converting sphingomyelin into ceramide and phosphorylcholine on membranes. Their activity has been linked to various neurological disorders, where altered lipid metabolism may contribute to disease progression. However, their role in Parkinson's disease (PD) remains unclear. By utilizing various model systems that mimic PD, focusing on the most common risk factor for PD mutations in *GBA1*, and extracellular vesicles (EVs), I am investigating how SMases contribute to disease progression. This is because understanding the role of SMases in EV subtypes that potentially carry toxic proteins in PD can reveal novel therapeutic targets to slow disease progression.

The image highlights immunostained HeLa cells treated with conduritol-beta-epoxide, an irreversible inhibitor of GCase, the enzyme encoded by *GBA1*. HeLa cells were transfected to overexpress nSMase (yellow) and an ER marker (mCherry-sec61b, magenta). The nSMase contains a C-terminal FLAG-tag, allowing detection with a FLAG M2 primary antibody and an anti-mouse secondary antibody. Results show nSMase outside the ER, potentially on the inner leaflet of the plasma membrane.

Why is your research important?

Exosomes have been extensively studied as potential carriers of pathological α-synuclein in PD, and their inhibition with certain drugs has been explored as a strategy to mitigate disease progression. However, targeting exosomes may inadvertently promote other vesicle subtypes that potentially carry α-synuclein. This highlights the need for a broader approach. By elucidating the role of SMases in EV production, our research aims to identify a novel therapeutic target(s), potentially offering a complementary approach to current treatments to slow disease progression for over 9 million Parkinson's patients worldwide.

Have you made any interesting findings in your research?

One subtype of sphingomyelinase, known as acidic sphingomyelinase (aSMase), is associated with lysosomal membranes and can be secreted to the plasma membrane under certain stressful conditions. This secretion process is thought to contribute to changes in membrane composition and extracellular vesicle formation. While increased levels of aSMase have been reported in several neurological disorders, its specific role in PD remains unclear. In a PD model system, we observed changes in aSMase activity using a biochemical assay alongside alterations in extracellular vesicle release. Additional imaging experiments revealed that inhibitors of sphingomyelinase activity reduced vesicle formation under these conditions, suggesting that aSMases may play a role in membrane dynamics and vesicle biogenesis in disease contexts.

What specific advice would you give to younger students who are interested in scientific research?

While it's important to choose a research topic that excites you, I believe the most crucial factor is finding the right team to work with. Research is inherently collaborative, and the people around you will shape your experience in profound ways. Take the time to meet the supervisor and lab members before committing to a lab to ensure the environment fosters growth.

For me, joining Dr. Ioannou's lab has been an incredibly rewarding experience. I'm deeply grateful for her guidance – her kindness, patience, and encouragement have made me mature both as a researcher and as a person. My lab mates have also been invaluable by always helping me troubleshoot experiments and brainstorm ideas. Being part of such a collaborative and supportive team has made my research journey rewarding.

If you could work in any laboratory in the world, what would you choose? What field of research would you want to be involved in?

I am passionate about innovative research that combines environmental sustainability with ecological health. As someone who practices/teaches worm composting and urban beekeeping, I am eager to explore two key areas: worm metabolism and bee population health.

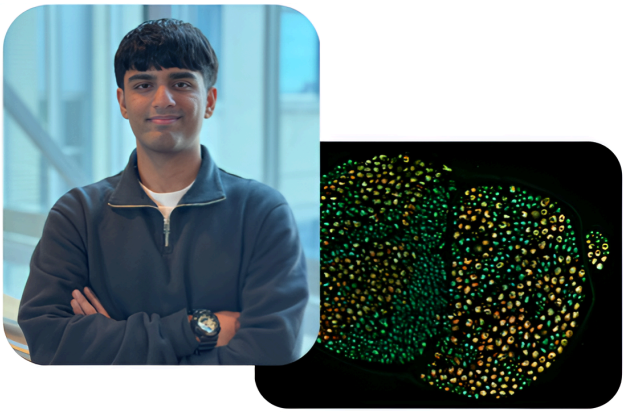
For worms, I aim to study the organic waste they process most efficiently, focusing on how diet influences their reproductive rates and composting effectiveness. This research could offer insights into addressing urban and agricultural waste challenges. In the realm of bees, I would love to research environmental factors driving the decline in bee populations. Investigating the impact of pollutants, pesticides, and climate change could lead to strategies that support bee recovery and enhance their vital role in pollination and food production.

Both areas of research are crucial in combating environmental challenges, and I would be grateful to contribute to solutions that foster sustainable ecosystems.

In regards to your research, who has influenced you the most?

In my research journey, no one has influenced me more than my supervisor, Dr. Julie Jacquemyn. She embodies resilience, intelligence, and dedication. Her unwavering positivity inspires me every day. Her innovative research techniques and profound knowledge have enriched my learning, but what stands out most is her emotional intelligence – she recognizes when I feel overwhelmed and provides thoughtful guidance that empowers me to persevere. Her ingenuity and perseverance in tackling challenges leave me in awe, and her motivation drives me to strive for excellence. I am incredibly grateful and honoured to learn from such an inspiring role model, and I hope to emulate her passion and strength in my own career.

Aryan and Taylor's image, titled *Mouse Radial Nerve in Cross-section*, is featured on the back cover of the issue. This triple fluorescent image highlights diverse axonal subpopulations using immunohistochemistry.



> "The most important aspect of science is to be able to embrace the failures you face when trying something new."

Tell us a bit about yourself!

I am Aryan Sharma, a fourth-year undergraduate student studying neuroscience. I joined the Webber Lab to deepen my understanding of peripheral nerve injuries and explore modern techniques for promoting regeneration. During a studentship this summer, I gained valuable insights into the various steps involved in data collection. Learning about the basic science underlying many clinical applications has encouraged me to pursue a career in medicine where I can eventually use my research to improve patient outcomes. Outside of school, I practice Muay Thai, go on hikes, read and experiment with cooking different cuisines.

What are the implications of your research?

Our research aims to improve our current understanding of the various sensory and motor axonal subpopulations that comprise peripheral nerves. These axons transmit sensory information regarding touch, pain, temperature and proprioception from the body to the brain, and relay motor signals from the brain to our muscles. Quantifying axonal subpopulations will enable us to explore novel animal models to study peripheral nerve regeneration post-injury. This research also has implications for surgical treatments of peripheral nerve injuries and improved therapeutic interventions for a patient's smooth recovery.

What interests you about this field?

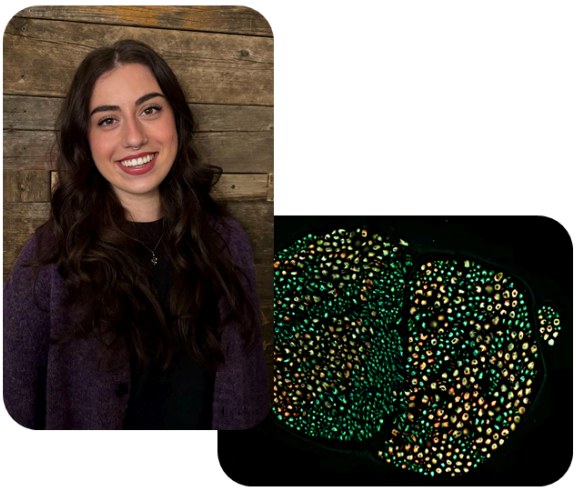
If there is one thing I love about neuroscience is that it is ever-evolving. Despite decades of research into the nervous system and its underlying physiology, we are still only scratching the surface of understanding its complexities. It is the excitement to uncover new pathways and structure-function relationships that motivates me to keep pushing forward, even if there are bumps along the way.

What have you learned from your research experience?

I feel like the most important aspect of science is to be able to embrace the failures you face while trying something new, whether it is a new protocol or new equipment. When we initially start out as scientists, we often get into research feeling confident about our data collection and experimental techniques. Over time, however, it becomes imperative to accept the learning curve that comes with a research project. During my time in the Webber lab, I have learned that these tiny obstacles that I may occasionally encounter while testing out my hypotheses are steps to ensure my experimental design is optimized for the project. This lesson is something that I have tried to incorporate into my daily life by responding to challenges with perseverance and grit.

What has been the most challenging part of your research experience thus far?

The most challenging aspect of my research experience so far has been troubleshooting protocols and refining them with each experiment. Although it can sometimes seem like a lot of work, this challenge has taught me the value of background literature as I often delve deep into the reasoning behind the various steps one has to take to complete an experiment. While addressing these challenges, I have also realized that I am not alone in this process. The wonderful advice from Dr. Webber and my fellow lab members is something that I can always count on.



Tell us a bit about yourself!

I am Taylor Mytko, a final-year undergraduate student studying biological sciences and psychology. My time in the Webber lab has ignited a deep interest in research and introduced me to the wonderful world of neuroscience. After graduation, I plan to pursue a career in veterinary medicine, driven by my passion for animals. My ultimate goal is to merge my love for animals with my research interests, contributing to advancements that improve the lives of our furry – or scaly – companions. Outside the lab, I enjoy spending quality time with friends and family, diving into a good book, caring for my snake, and unwinding through yoga or a nice long walk.

Why is your research important?

Peripheral nerve injuries cause immense physical and emotional distress to patients and their families. Even though peripheral nerves can regenerate, the process is extremely slow and function is not always restored. Our research aims to quantify and compare the basic sensory and motor axonal subpopulations across a variety of upper and lower limb peripheral nerves. This will provide us with a baseline upon which injury models can be developed to further study the regeneration rate of fiber subtypes. This type of information may assist clinicians in choosing the most appropriate donor nerve during nerve transfer surgery, ultimately improving patient recovery outcomes following a peripheral nerve injury.

What interests you about this field?

I am particularly drawn to neuroscience and the research we conduct in the Webber lab because of its potential for meaningful clinical applications. We get the opportunity to collaborate with clinicians, bridging the gap between basic science and patient care. Knowing that the research we perform in the lab can directly contribute to improving patients' quality of life is both inspiring and rewarding.

"Learning to accept unexpected results or failed experiments as opportunities for growth is crucial."

What have you learned from your research experience?

The knowledge and insights I have gained from my research experience are truly invaluable and limitless. One key takeaway has been the realization that things rarely go as planned, and it's important not to have rigid expectations. As Dr. Webber often says, science is hard – and if it weren't, everyone would be doing it. Learning to accept unexpected results or failed experiments as opportunities for growth is crucial. These moments not only improve the quality of your research but help you grow as a scientist in the making. Ultimately, my research experience has taught me resilience and adaptability, qualities that are essential for success in both research and life.

What has been the most challenging part of your research experience thus far?

As a biological sciences student not specializing in any particular domain, entering a neuroscience lab was initially intimidating. I felt as though I had years of catching up to do or wasn't qualified to contribute to the research. However, reading relevant literature and seeking guidance from my supervisor and lab mates helped build my confidence. I quickly realized that everyone starts somewhere, and if I hadn't stepped out of my comfort zone, I never would have discovered my passion for neuroscience and research. Although the work in the lab can be challenging, overcoming self-doubt proved to be an even greater hurdle.

eureka Research article

Representing The World Around Us: Applications of Group Representation Theory to Molecular Orbital (MO) theory

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ABSTRACT

Molecular orbital (MO) theory is at the forefront of modern chemistry, allowing for accurate descriptions of the reactivity of molecules by using quantum mechanics to predict the location and energies of electrons within a molecule. The equations which govern their behavior, the Schrodinger equation, are often difficult to solve. Sometimes, we can only approximate a solution using numerical methods. This paper discusses a method that exploits a molecule's internal symmetry. Specifically, we use Group representation theory to help analyze and break down the molecular symmetry, and then use the analysis to help us find the MOs. First, we establish key results about irreducible representations and characters. We then establish a correspondence between MO's and irreducible representations. We then use the results obtained to perform MO calculations on water. We then compare the results obtained via our MO theory calculations and Valance Bond Theory (VBT). We conclude by showing these calculations are best used for rough work, being most useful for deciding which atomic orbitals they arose from, and each MO's energies relative to each other.

KEY WORDS: **Molecular Orbital (MO) theory, Group theory, Representation Theory, Symmetry-Adapted Linear Combination (SALC), Quantum Chemistry**

1 | INTRODUCTION

Molecular orbital (MO) theory is a theory in chemistry that describes the nature of chemical bonding. It assumes that all atoms that constitute a larger molecule combine their atomic orbitals to construct larger MOs (Galbraith et al., 2021). In essence, orbitals are 'regions of electron density.' These regions of density are dictated by the electron's wave function(s), which in turn are governed by the Schrodinger equation, given by (Miessler et al., 2022)

$$\hat{H}\psi = E\psi$$

where $\hat{H}$ is the Hamiltonian operator, ψ is our wave function, and E is the energy (eigenvalue) of the wave function. Solving it is quite difficult, as it typically involves second-order Partial Differential Equations (PDEs) with complicated boundary conditions. Sometimes, all we can do is approximate solutions. However, solutions to this equation allows us to gain insight into a molecule's electronic structure and thus its reactivity and is thus of great significance to chemists.

1.1 Group Theory and Abstract Algebra

Abstract algebra is a branch of mathematics which aims to study algebraic structures, like Groups, Rings, &Fields (Carter, 2021). This paper focuses on groups and their applications to problems in Chemistry, but they also appear in physics and computer science, among other disciplines (Carter, 2021).

At its core, Group theory is mathematical study of an object's symmetries (Carter, 2021). Before formally defining

what groups are, we consider an example (Figure 1). Notice how we can combine 2 subsequent symmetries of the square to obtain another: for instance, if we reflect along the x axis, then reflect along the y axis, this is the same as rotating the square 180 degrees counterclockwise. There is also a way to 'undo' each symmetry: if you turn 90 degrees clockwise, turning counterclockwise 90 degrees undoes the original turn. Lastly, there is a 'home state': the configuration shown above. The set of symmetries associated with this square form a group (under composition).

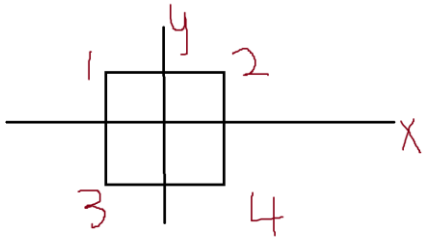

Figure 1: Square on the x-y plane, centered at the origin [self-generated]

Formally speaking, a group is a set G with a binary operation $*$ [a function/rule which takes pairs of elements in G and returns some element in G, with $*(a, b)$ denoted $a * b$ which satisfies the following properties:

1. There exists an identity element (typically denoted e) which satisfies $e * a = a = a * e$ for every $a \in G$
2. This binary operation is associative $a * (b * c) = (a * b) * c$ for any $a, b, c \in G$
3. Every element has an inverse: for every $a \in G$, there exists some $a^{-1} \in G$ such that $a * a^{-1} = a^{-1} * a = e$

Of course, we have only really scratched the surface of group theory and abstract algebra, with more details relegated to the appendix.

1.2 Representation Theory

Informally, representation theory is a way to associate elements of a group G to invertible matrices in such a way which preserves the group's algebraic structure. This allows us to use the tools of linear algebra and the mathematical theories associated with vector spaces to study our group G by encoding symmetries in terms of matrices. More formally, we define a representation of a group G as follows (Serre, 1977):

Definition 1*. A representation of a group G is a map $\rho: G \to GL(V)$ which is a homomorphisim [a homomorphism is a function between 2 groups which preserves the algebraic structure], Where $GL(V)$ denotes the group of invertible linear maps from a vector space V to itself. V is called the representation space.*

Here, if group theory and linear algebra are 2 different mathematical 'languages', then ρ behaves like a translator between the 2 'languages' and allows us to go between them. For simplicity, assume that all groups are finite, and that our vector spaces are complex and finite dimensional. This allows us to associate elements $g \in G$ to an invertible $n \times n$ matrix ρ_g with complex number entries, where $n < \infty$. In short, representation theory is a way to encode an object's symmetries in terms of matrices and linear algebra.

One important notion within representation theory is that of subrepresentations. These are representations which act on subspaces of the representation space V which are 'invariant' under the representation. By studying these sub-representations, we can use them to understand the whole. We formalize this notion as follows (Serre, 1977):

Definition 2*. Let G be a group and let $\rho: G \to GL(V)$ be a representation. Then W is a subrepresentation of G if*

1. *W is a subspace of V.*
2. *for any $g \in G$, we have that $\rho_g(W) \subseteq W$ (that is, elements in W get mapped to other elements in W under any ρ_g, and thus W is 'invariant').*

If the only such subspaces are $\{0\}$ and V itself, then our representation is said to be irreducible. Irreducible representations, sometimes called irreps or irreducibles, play a role analogous to that of prime numbers in $\mathbb{Z}$. Just like how an integer can be written as a product of prime number powers, we will show every representation can be written as a direct sum of (some number of copies of) irreducibles. Moreover, knowing an integer's prime factorization gives us information about that number, like its gcd (greatest common divisor) and lcm (lowest common multiple). Similarly, we will see that irreducible representations give us insight into a molecule such as the degeneracy of an MO, its relative energies, and which AOs formed it (Lowe & Peterson, 2011).

There are many representations of a group. However, it might be possible that two representations of G might end up encoding the same information, just in different ways. For instance, consider the representations ρ, ρ' of the group $C_2 = \{e, a\}$, where $a^2 = a * a = e$, given by:

$$p(a) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, p'(a) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

Both ρ and ρ′ encode a reflection but do it differently: ρ about the x axis, and ρ′ about the y axis. This notion of two different things having the same algebraic structure, and thus encoding the same information is an important mathematical idea known as isomorphism (Serre, 1977). In the context of group representations, isomorphism is defined as follows (Serre, 1977):

Definition 3*. Let $\rho: G \to GL(V)$, and $\rho': G \to GL(V')$ be two representations of G. we say that $\rho \cong \rho'$ [that is, ρ is isomorphic to ρ'] if there exists some invertible linear map $T: V \to V'$ such that for every $g \in G$, we have that:*

$$T \circ \rho_g \circ T^{-1} = \rho'_g$$

An important remark here is that this map T is the same for all the ρ_g. This notion, called simultaneously similar, is a stronger requirement than simply requiring each ρ_g to be similar to the ρ'_g, since we use the same 'similarity' matrix for all of them.

1.3 MO theory

To talk about MO theory, first, we need to talk about Atomic Orbitals (AO's), and our understanding of the atom. Our modern understanding of the atom consists of three types of particles: protons and neutrons packed together inside of a densely packed nucleus, with electrons flying around this nucleus (Sullivan & Musgrove, 2023). As our understanding of quantum mechanics started to improve, we could now predict where electrons were located within the atom. The wave nature of the electron gives a corresponding wave function that describes its behavior (Sullivan & Musgrove, 2023), which can be obtained by solving the following equation (Miessler et al., 2022):

$$\hat{H}\psi = E\psi$$

Where $\hat{H}$ is the Hamiltonian operator, ψ the wave function and E is the energy. The wave function ψ itself has no direct use, but $\psi * \overline{\psi} = ||\psi||^2$ does, being interpreted as the probability of finding an electron within a certain region of space/'electron density map.' These regions of electron density generated by $||\psi||^2$ are called orbitals. Although 'wavefunction' and 'orbital' are technically different, they will be used interchangeably.

Within an energy level, the angular momentum of electrons gives rise to sublevels, denoted s, p, d, and f (Sullivan & Musgrove 2023). In terms of their energies, we have s<p<d<f. These sublevels are shown in Figure 2.

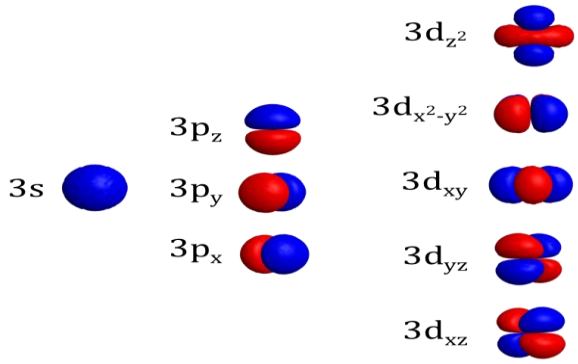

Figure 2: Various atomic orbitals [obtained (with permission to reproduce) from (Kennephol, n.d.)]

From the picture, we can observe some various symmetry within the sublevels, arising from the electron's angular momentum. For instance, the s orbital possesses spherical symmetry, and the p orbitals have a dumbbell-symmetry to them.

When atoms combine to create molecules, the highest energy atomic orbitals (valance orbitals) will overlap with each other to form MO's (Miessler et al.,2022). We aim to use representation theory to establish a correspondence between irreducible representations and these MO's.

2 | METHODS

Mathematical proof is the primary method of analysis for this paper. We first prove key results from representation theory concerning sub-representations and character theory. Then, we establish a correspondence between MO's and irreducible representations, before finally working through an example (a water molecule) of how we can use the SALC method to perform MO calculations.

To prove these results, we mostly use tools from linear algebra and a bit of group theory. While efforts to keep things accessible have been made, familiarity with the following linear algebra topics is ideal: span, linear independence, orthogonality in $\mathbb{R}^n$, projections, linear transformations, inner product spaces, spectral theory, Jordan normal form, and have some exposure to direct sums/tensor products. In addition, some knowledge of group theory is also useful:

knowledge of what groups are, their properties, homo/isomorphisms, conjugacy & the class equation.

3 | RESULTS

First, we (re)address some assumptions we make for this section: assume our groups G are of finite order, and vector spaces are finite-dimensional and complex, so we can associate elements $g \in G$ to an invertible $n \times n$ matrix ρ_g with complex number entries, with $n < \infty$. The goal of this section is to establish some results from representation theory needed to perform MO calculations, listed below:

1. Every representation has a decomposition into irreducibles.
2. Characters on irreducible representations give an orthonormal basis (which we need to find the above decomposition)

3.1 The role of irreducible representations

The goal of this subsection is to establish the first result on the above list. More formally, we can write that statement as follows:

Theorem 4 *(Maschke's theorem): Every representation is either irreducible or can be decomposed into a direct sum of irreducible representations (Serre, 1977).*

To prove this, we need to create subspaces which are invariant under the action of G (a subrepresentation). However, given some subrepresentation W, we can make another subrepresentation by averaging out the projection onto W over the group G. The following lemma goes through the details of this process (Serre, 1977):

Lemma 5*. Let $\rho: G \to GL(V)$ be a representation of G, with representation space V, and a subrepresentation W. Then there exists some subspace W^C is also stable under the action of G (a subrepresentation) and satisfies $V = W \oplus W^C$.*

3.2 Proof of Lemma 5 [Adapted from (Serre, 1977)]:

First, let P be some projection from V onto W, and we use it to define a map, P°, which 'averages' the projection map over G:

$$P^\circ(x) = \left[\frac{1}{|G|}\sum_{g\in G} \rho_g \, P \rho_g^{-1}\right] x$$

We claim P° is a projection onto W. First, we show that that $P^\circ(x) = x$ for any $x \in W$ and any $g \in G$. Indeed, if we fix some $x \in W$ and $g \in G$, we see the result outlined below:

$$P^\circ(x) = \left[\frac{1}{|G|}\sum_{g\in G} \rho_g \, P \rho_g^{-1}\right] x$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_g \left(P\left(\rho_g^{-1}(x)\right)\right) = \frac{1}{|G|}\sum_{g\in G} \rho_g \left(\rho_g^{-1}(x)\right)$$

$$= \frac{1}{|G|}\sum_{g\in G} x = \mathrm{x}$$

Moreover, we remark that:

1. P° maps from V to W (since P is a projection onto W any $x \in V$ implies $P(x) \in W$, and W is an invariant subspace of ρ_g , so for all $x \in W$, we have $\rho_g(x) \in W$).
2. P° is the identity on W (since $P^\circ(x) = x$ for any $x \in W$).

Thus, we have that P° is a projection from V to W, for which it is the identity on W. Thus P° is a projection onto W. We also observe that for any $h \in G$, we have that $\rho_h P^\circ \rho_h^{-1} = P^\circ$ as we see that:

$$\rho_h P^\circ \rho_h^{-1} = \rho_h \left[\frac{1}{|G|}\sum_{g\in G} \rho_g \, P \rho_g^{-1}\right] \rho_h^{-1}$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_h \, \rho_g P \rho_g^{-1} \rho_h^{-1}$$

$$= \frac{1}{|G|}\sum_{g\in G} \rho_{hg} \, P \rho_{hg}^{-1}$$

$$= P^\circ$$

Since we have $\rho_h P^\circ \rho_h^{-1} = P^\circ$, it follows that $\rho_h P^\circ = P^\circ \rho_h$ for any $h \in G$. Thus, we take our new subrepresentation W^C to be $ker\ (P^\circ)$. This subspace is indeed stable under the action of G, since for any $y \in W^C$ and any , $g \in G$ we see that:

$$P^\circ\left(\rho_g(y)\right) = \rho_g\left(P^\circ(y)\right) = \rho_g(0) = 0$$

$$\Longrightarrow P^\circ\left(\rho_g(y)\right) = 0$$

Thus, for any $g \in G$ and any $y \in W^c$, we have $\rho_g(y) \in W^c$. Lastly, because P° is a projection, we have that $V = ker(P^\circ) \oplus Im(P^\circ)$. Since we defined W^c to be the kernel of P°, and the image of P° is W, we have that $V = W \oplus W^C$. This completes the proof. This completes the results needed to prove theorem 4, done below.

3.3 Proof of Theorem 4: Maschke's theorem

This is again adapted from (Serre, 1977), proceeding by induction on $\dim(V)$. The base case of $\dim(V) = 0$ gives the 0-space, which is irreducible. To see this, consider what the subspaces of the 0-space are.

Now, suppose that we can decompose V into a direct sum of irreducible subrepresentations if $\dim(V) \leq n$, and we consider what happens if $\dim(V) = n + 1$. If V is irreducible, then there is nothing to check since it is irreducible. If V is reducible, then we have a proper subrepresentation W, and can apply Lemma 5 to find a subrepresentation W^c such that $V = W \oplus W^c$. Since W, W^c are subrepresentations and V is reducible they must be proper subspaces of V. Thus, we have that $\dim(W) < \dim(V)$ & $\dim(W^C) < \dim(V)$ and apply the induction hypothesis on W, W^c to complete the proof.

Thus, we have that every representation has a decomposition into irreducibles, analogous to how every integer has a prime factorization. However, we have not addressed how one finds a decomposition. Character theory seeks to address this issue.

3.4 Character Theory

Having established that we can decompose a representation into irreducibles, we aim to find a way to compute them. To do this, we need to introduce the notion of the character of a representation, defined below (Fulton & Harris, 2004):

***Definition 6**. The Character χ_ρ of a representation ρ is a map from our group G to $\mathbb{C}$ given by $\chi_\rho(g) = Tr(\rho_g)$, where $Tr(M)$ denotes the trace of a square matrix M, the sum of diagonal entries.*

Trace is invariant under similarity of matrices. Thus, isomorphic representations have equal characters. However, this goes both ways, as representations that have equal characters are isomorphic (Schedler, n.d.). Thus, characters can be used to uniquely identify a representation of a group up to isomorphism.

When the context is clear, subscripts are dropped, with χ_ρ becoming χ. Moreover, if the representation is irreducible, its associated character is also said to be irreducible (Serre, 1977).

Given representations $\rho: G \to V, \rho': G \to GL(V')$, one can define direct sums $\rho \oplus \rho'$ by the map $\rho \oplus \rho': G \to V \oplus V'$ by sending $g \in G$ to the map which sends $(v, w) \in V \oplus W$ to $\left(\rho_g(v), {\rho'}_g(w)\right)$. One can also define $\rho \otimes \rho'$ in an analogous way on pure tensors. For dual spaces, one can define the dual of a representation ρ^* by $\rho^*(g) = \left(\rho_g^{-1}\right)^T$ on V^* (Fulton & Harris, 2004).

The following proposition establishes some basic properties of characters on direct sums and tensor products (Fulton & Harris, 2004).

***Proposition 7**. let $\rho: G \to GL(V), \rho': G \to GL(V')$ be representations of G. Then we have that*

1. $\chi_{\rho \oplus \rho'} = \chi_\rho + {\chi_\rho}'$
2. $\chi_{\rho \otimes \rho'} = \chi_\rho * {\chi_\rho}'$
3. $\chi_{\rho^*} = \overline{\chi_\rho}$

Another property characters have is that group elements in the same conjugacy class have equal character, since if we have $a, b, g \in G$ such that $a = gbg^{-1}$ then:

$$\chi_\rho(a) = \chi_\rho(gbg^{-1}) = Tr(\rho_{gbg^{-1}})$$
$$= Tr\left(\rho_g(\rho_b\rho_{g^{-1}})\right) = Tr\left((\rho_b\rho_{g^{-1}})\rho_g\right)$$
$$= Tr(\rho_b) = \chi_\rho(b)$$

Characters are thus constant on conjugacy classes, & are dubbed class functions (Serre, 1977). The set of all class functions associated with a fixed group G, C_G form a complex inner product space (Serre,1977), with addition/scalar multiplication is done pointwise, and the inner product given by (Serre, 1977):

$$\langle \chi_\rho, {\chi_\rho}' \rangle = \frac{1}{|G|} \sum_{g \in G} \overline{\chi_\rho(g)}\, {\chi_\rho}'(g)$$

Here, an inner product aims to give rise to the notion of distances and angles within an abstract vector space (Axler, 2024). In particular, this inner product gives us a way to talk about the length of a character or angles between 2 characters. Verification of all the relevant properties amounts to routine calculations and is thus left to the reader.

Since characters are class functions, if G has k conjugacy classes, we can index the sum by the conjugacy classes, and rewrite the inner product as:

$$\langle \chi_\rho, \chi_\rho{}' \rangle = \frac{1}{|G|} \sum_{i=1}^{k} n_i \overline{\chi_\rho(g_i)} \chi_\rho{}'(g_i)$$

where n_i denotes the number of elements in each conjugacy class, and g_i some representative.

Having now established what characters are, and some of their key properties, we work to prove the following:

Theorem 8*. Characters of irreducible representations (irreducible characters) form an orthonormal basis [a basis which all basis vectors are orthogonal to each other and have length 1] for* C_G.

However, we need to establish some preliminary results. The first of these gives a formula relating the dimension of a representation and its character (Fulton & Harris, 2004).

Lemma 9*. Let* $\rho: G \to GL(V)$ *be a representation with subrepresentation* $V^G = \{v \in V | \rho_g(v) = v \text{ for all } g \in G\}$, *and define a linear map* $\phi: V \to V$ *by* $\phi(v) = \frac{1}{|G|} \sum_{g \in G} \rho_g(v)$. *Then* ϕ *is a projection from* V *onto* V^G.

3.5 Proof of Lemma 9 [adapted from (Fulton & Harris, 2004)]:

We first show that $V^G = \mathrm{Im}(\phi)$, from which it follows V^G is a subrepresentation [when we prove Schur's lemma later, we will see that images of linear maps are subrepresentations]. We note that for any $v \in V^G$ we can observe that:

$$v = \frac{1}{|G|}|G|v = \frac{1}{|G|}\sum_{g \in G} v = \frac{1}{|G|}\sum_{g \in G} \rho_g(v) = \phi(v)$$

The 3rd equality is a result of rewriting $|G|$ as the sum of $|G|$ many 1's, and the fact that for any $g \in G$ *and* $v \in V^G$, *we have* $\rho_g(v) = v$. This shows that $\mathrm{Im}(\phi) \supseteq V^G$. For the other inclusion, let $v \in V$, and we show that $\phi(v) \in V^G$. Indeed, for any $h \in G$, we have that:

$$\rho_h(\phi(v)) = \rho_h\left(\frac{1}{|G|}\sum_{g \in G} \rho_g(v)\right) = \frac{1}{|G|}\sum_{g \in G} \rho_h\left(\rho_g(v)\right)$$
$$= \frac{1}{|G|}\sum_{g \in G} \rho_{hg}(v) = \phi(v)$$

Where the 2nd equality holds comes from distributing the matricies, the 3rd one is a result of ρ being a group homomorphisim, and the last equality holds as the h simply re-orders the terms in the sum. This gives us the desired equality of sets.

To show that $\phi \circ \phi = \phi$, all that one needs to do is evaluate the quantity $\phi(\phi(v))$. The resulting double sum is straightforward but requires substantial amounts of calculation, so we leave it to the reader. Since ϕ is a projection, we have that $\dim(Im(\phi)) = Tr(\phi)$. To see this, consider the Jordan normal form, ϕ_J of ϕ. Since ϕ is a projection, there are 2 eigenvalues of ϕ: 0 and 1. For the Jordan block associated with eigenvalue 1, the eigenspace associated with it is just V^G, and consequently, the Jordan block for the eigenvalue 1 is simply the identity matrix of size $dim(V^G)$. For the block associated with eigenvalue 0, it is simply the 0 matrix of size $dim((V^G)^c)$, where $(V^G)^c$ is the orthogonal complement of V^G. We note that since $\mathrm{Im}(\phi) = V^G$, it follows that they agree in dimension, so we get $\dim(V^G) = dim\left(im(\phi_J)\right)$. Lastly, the trace of ϕ and ϕ_J are the same, as they are similar matrices. Thus, we have that $\dim(V^G) = \dim(\mathrm{Im}(\phi)) = \dim\left(\mathrm{Im}(\phi_J)\right) = \mathrm{Tr}(\phi_J) = Tr(\phi)$.

We note that since $\mathrm{Im}(\phi) = V^G$, it follows that they agree in dimension. Thus, we observe that:

$$\dim(\mathrm{Im}(\phi)) = \dim(V^G) = Tr(\phi)$$
$$= Tr\left(\frac{1}{|G|}\sum_{g \in G} \rho_g\right) = \frac{1}{|G|}\sum_{g \in G} Tr(\rho_g) = \frac{1}{|G|}\sum_{g \in G} \chi_\rho(g)$$

and thus obtain the formula below (denoted formula 4.1).

$$\dim(V^G) = \frac{1}{|G|}\sum_{g \in G} \chi_\rho(g)$$

We now prove the next lemma, aiming to classify the possible maps which go between any two irreducible representations:

Lemma 10 *(Schur's lemma). Let* $\rho: G \to GL(V), \rho': G \to GL(V')$ *be two different representations of a group* G *which*

are both irreducible and let $f: V \to V'$ be a linear map such that for any $g \in G$, we have $f \circ \rho_g = \rho'_g \circ f$. Then

1. *if $\rho \ncong \rho'$, then $f \equiv 0$*
2. *if $\rho \cong \rho'$ and $V = V'$, then $f = cI$, where I denotes the identity map, and c is a constant.*

3.5 Proof of Lemma 10 [adapted from (Serre, 1977)]:

We prove each part separately. To prove the first part of Schur's lemma, we first need to show that $\ker(f)$ and $\mathrm{Im}(f)$ are G-invariant subspaces. For any $y = f(x) \in \mathrm{Im}(f)$, we see that

$$\rho'_g(y) = \rho'_g\big(f(x)\big) = f\left(\rho_g(x)\right)$$

$$\Longrightarrow \rho'_g(y) \in \mathrm{Im}(f) \ \text{[Since } \rho_g(x) \in V\text{]}$$

and thus $\mathrm{Im}(f)$ is a subrepresentation. Similarly, for any $x \in ker(f)$, we see that:

$$f\left(\rho_g(x)\right) = \rho'_g\big(f(x)\big) = \rho'_g(0) = 0 \Longrightarrow \rho_g(x) \in ker(f)$$

This shows that $\ker(f)$,$\mathrm{Im}(f)$ are sub-representations of G (that is, they are G-invariant). Now, consider the chain of inclusions below:

$$\{0\} \subseteq \ker(f) \subseteq V$$
$$\{0\} \subseteq \mathrm{Im}(f) \subseteq V'$$

Since ρ, ρ' are irreducible, the only possibilities for $ker(f)$ and $\mathrm{Im}(f)$ are either $V = ker(f)$ and $\mathrm{Im}(f) = 0$ or $ker(f) = \{0\}$ and $\mathrm{Im}(f) = V'$. But $ker(f) = \{0\}$ and $\mathrm{Im}(f) = V'$ would imply f is invertible. Thus, from the fact that $f \circ \rho_g = \rho'_g \circ f$, we can obtain that $f \circ \rho_g \circ f^{-1} = \rho'_g$, for any $g \in G$, contradicting the assumption $\rho \ncong \rho'$. Thus $V = ker(f)$ which gives $f = 0$.

To address the second part, suppose that $\rho \cong \rho'$ and $V = V'$, and let $f: V \to V$ be linear. Since $\mathbb{C}$ is algebraically closed [every polynomial with complex coefficients has a complex root], f must have some eigenvalue λ. Thus, set $h = f - \lambda I$, and it follows that for any $g \in G$, we have $h \circ \rho_g = \rho'_g \circ h$. To see this, substitute h into one side, and make use of the fact $f \circ \rho_g = \rho'_g \circ f$ and $\lambda I \circ \rho_g = \rho'_g \circ \lambda I$. Since f has an eigenvalue, we have that $ker(h) \neq 0$. Thus, by the previous point, we must have that $h = 0$, from which it follows $f = \lambda I$.

Thus, given two irreducible representations $\rho: G \to GL(V)$ and $\rho': G \to GL(V')$, Schur's lemma allows us to give an explicit description of elements in the set $Hom_G(V, V')$. Here, $Hom_G(V, V')$ is the set of all linear maps $T: V \to V'$ which obey $\rho'_g \circ T = T \circ \rho_g$ for any $g \in G$ [that is, these maps intertwine/ "translate between" representations ρ & ρ′]. If $\rho \ncong \rho'$, then the only possible $T \in Hom_G(V, V')$ by part 1 of Schur's lemma is the 0 map, & $Hom_G(V, V') = \{0\}$.

If, $\rho \cong \rho'$ however, then any nonzero $\theta \in Hom_G(V, V')$ is invertible. Thus, for any nonzero maps $\phi, \theta \in Hom_G(V, V')$, we have that $\theta^{-1} \circ \phi \in Hom_G(V, V)$. But part 2 of Schur's lemma gives us that $\theta^{-1} \circ \phi = cI$ for some $c \in \mathbb{C}$. Thus, we compose by θ on both sides to obtain $\phi = c\theta$ (Chua, n.d.). We conclude that $Hom_G(V, V') = span\{\phi\}$ for some invertible linear map $\phi: V \to V'$ on irreducible representations. In short, we have that:

$$Hom_G(V, V') \cong \mathbb{C} \text{ if } \rho \cong \rho' \text{ and } \{0\} \text{ otherwise}$$

Given that $Hom_G(V, V') \cong V^* \otimes V'$ (Fulton & Harris, 2004), we have that $\chi_{Hom_G(V,V')} = \overline{\chi_\rho}\chi_{\rho'}$ by proposition 7. Since isomorphic vector spaces have the same dimension, we can apply formula 4.1, to obtain the following:

$$\dim\big(Hom_G(V, V')\big) = \frac{1}{|G|}\sum_{g \in G} \chi_{Hom_G(V,V')}$$
$$= \frac{1}{|G|}\sum_{g \in G} \overline{\chi_\rho(g)}\,\chi_{\rho'(g)}$$

Where χ_ρ is the character of $\rho: G \to GL(V)$, and $\chi_{\rho'}$ is the character of $\rho': G \to GL(V')$. Combining this with the observation that $\dim(Hom_G(V, V')$ is either 0 or 1 (on irreducible representations), by our above work, we get that:

$$\frac{1}{|G|}\sum_{g \in G} \overline{\chi_\rho(g)}\,\chi_{\rho'(g)} = 1$$
$$\text{[if } \rho \cong \rho' \text{ and is 0 otherwise]}$$

This work shows that the set of irreducible characters forms an orthonormal set in C_G, implying linear independence. Moreover, Theorem 4 shows that every representation can be decomposed into irreducibles, so the set of irreducible characters also forms a spanning set in C_G. Thus, the set of irreducible characters forms an orthonormal basis for C_G, which was precisely theorem 8.

Given our orthonormal basis, one can easily compute the decomposition into irreducibles by projecting onto each irreducible. This process is formalized below as proposition 11.

Proposition 11*. If ρ is a representation of a finite group G with character χ, and we have $\rho = \bigoplus_{i=1}^{k} m_i\rho_i$, with all ρ_i*

irreducible, and m_i *positive integers, then* $m_i = \frac{1}{|G|}\sum_{g\in G} \overline{\chi_\rho(g)}\,\chi_{\rho_i}(g)$ *for any* $1 \le i \le k$.

These scalars associated with the irreducible representations are called the multiplicities of an irreducible representation (Fulton & Harris, 2004). They give the 'number' of copies or times a certain irreducible representation occurs in our representations. Going back to the prime number analogy on page 4, they are analogous to the exponents in a prime factorization. Like with prime factorization, we ignore the irreducibles of multiplicity 0.

3.6 Proof of Proposition [adapted from (Bouchard, 2020)]:

Given that $\rho = \bigoplus_{i=1}^{k} m_i \rho_i$, we have that $\chi = \sum_{i=1}^{k} m_i\,\chi_i$. To this equation, we take the inner product of both sides with some fixed χ_j, and obtain that.

$$\langle \chi, \chi_j \rangle = \left\langle \sum_{i=1}^{k} m_i \chi_i \chi_j\,, \chi_j \right\rangle$$

$$= \sum_{i=1}^{k} m_i \langle \chi_i, \chi_j \rangle = m_j \langle \chi_j, \chi_j \rangle = m_j$$

Where the 2nd equality comes from the linearity of the inner product, and the 3rd the fact that $\langle \chi_i, \chi_j \rangle = 1$ if $i = j$ and is 0 otherwise. Thus, we obtain the following formula below

$$m_j = \langle \chi, \chi_j \rangle = \frac{1}{|G|}\sum_{g\in G} \overline{\chi_\rho(g)}\,\chi_{\rho_j}(g)$$

In the Chemistry context, this formula for the m_j is known as the 'reduction formula' (Miessler et al., 2022).

3.7 Chemical Results

Now that we have finished proving all the necessary mathematical results, we can start to put the pieces together. The goal of this section is to prove one more result (Lowe & Peterson, 2011):

Theorem 12*. One can associate each MO of a molecule with some irreducible representation of a molecule's point group.*

The importance of this theorem cannot be understated: This theorem allows us to deduce information about an MO, such as which atomic orbitals were used to form it, its relative shape, and energies by only knowing with which irreducible representation it is associated.

Before continuing, we first need to incorporate a group structure into our molecule. Fortunately, this is easy since many molecules have internal symmetry. For instance, take water, H_2O, pictured in Figure 3.

From left to right, we have an axis of rotation (labelled C_2), and the 2 internal planes of reflection. This set of symmetries forms a group under composition. This group of internal symmetries is called the point group of a molecule (Miessler et al., 2022), as we treat the atoms as points in 3d space centred about some fixed point. Typically, the 'central atom' of a molecule is the fixed point and is thus associated with the origin.

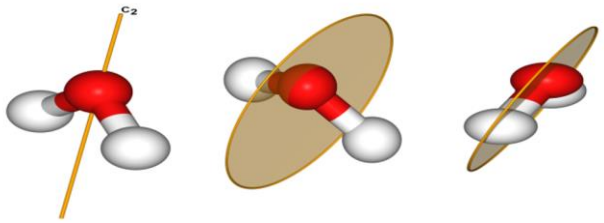

Figure 3: Water molecule with its various symmetries highlighted [obtained from (University, n.d.), with permission to reproduce]

In the case of water, all our symmetries above 'fix' the oxygen (red) atom, so we take it to be the origin. Convention also dictates that the main axis of rotation of a molecule (in the case of water, the C_2 axis) is the Z axis (Miessler et al., 2022).

We remark that since the MOs make up the molecule (and thus it is internal symmetry), we have that the set of all MOs for a given molecule is invariant under a molecule's point group. Put another way, the group of symmetries associated with the set of a molecule's MOs is the same as that molecule's point group. This observation is significant since finding a point group of a molecule is much easier than finding all a molecule's MOs (we will see this in the next section). Thus, by knowing the symmetries of the molecule, we know the symmetries of all our MOs. Thus, we can build a representation of this group of symmetries and thus can use the tools outlined in the previous sections to break that representation down and understand it. Theorem 12 will allow us to contextualize the results we have established about group representations in terms of our MOs.

Before proving Theorem 12, we need some more groundwork related to solutions to the Schrodinger equation, and general assumptions used in quantum mechanics: firstly, when we talk about things like the "norm of a wave function", we assume this norm is calculated with respect to the usual

inner product on complex-valued functions on some domain S, $C(S)$, given by

$$\langle f, g\rangle = \int_S f(x)\overline{g(x)}dx$$

we also need to introduce the concept of degeneracy, defined below (Lowe & Peterson, 2011):

Definition 13*. 2 different orbitals (wave functions) are said to be degenerate if they are in the same energy level.*

If there are more than 2 degenerate orbitals, then the number of orbitals in a given energy level is called the degeneracy. Since orbitals are simply the square of wavefunctions, and these wavefunctions are eigenfunctions of the Hamiltonian operator (associated with some eigenvalue E), we can equivalently define degeneracy as the dimension of the eigenspace associated with E. We assume without loss of generality that these wavefunctions form an orthonormal set (if not, just apply Gram-Schmidt algorithm). With that, we are now ready to prove theorem 12.

3.8 Proof of Theorem 12 [Adapted from ("Molecular orbital theory and its symmetry 393 aspects", n.d.), (Vvednsky, n.d.)]:

The first thing one needs to show is that the Hamiltonian is invariant under each symmetry operation (Vvednsky, n.d.): that is, if R is some element in your point group, we have that $R\widehat{H} = \widehat{H}R$. The symmetry operations only interchange identical nuclei, and thus permute wavefunctions (by the symmetry of the molecule). From this, it follows that the Hamiltonian is invariant under our point group.

Thus, if ψ is the wave function associated with your orbital, it is an eigenfunction of the Hamiltonian. From the fact that $\widehat{H}$ and R commute, we conclude that $R\psi$ is also an eigenfunction of $\widehat{H}$, so we set $R\psi = c\psi$, where c is some constant. From here, we treat the cases of non-degenerate and degenerate wavefunctions separately.

In the case of a non-degenerate wave function, then the normalization conditions imposed on the wave function (the wave function has norm 1) imply that $R\psi = \pm\psi$, since if $R\psi = c\psi$ for some constant c, we have that

$$\langle c\psi, c\psi\rangle = 1 \Longrightarrow |c|^2\langle\psi,\psi\rangle = 1$$
$$\Longrightarrow |c|^2 = 1\,(\psi \text{ has norm } 1) \Longrightarrow c = \pm 1$$

Since $c\psi\overline{c\psi}$ is real-valued, and the group operations only re-orient $c\psi\overline{c\psi}$, and do not change the area enclosed by it, we have that $c \in \mathbb{R}$. (Lowe & Peterson, 2011). Thus, $|c|^2 = c^2$.

Thus, it follows that the wave function is either symmetric or anti-symmetric with regard to any symmetry operation of our point group. If it is symmetric, then the eigenvalue is +1, and if it is anti-symmetric, it is -1. Thus, an easy representation can be constructed by the matrices [1] and [-1], associating elements that are symmetric to [1], and those which are anti to [-1]. Notice how this representation is 1-dimensional and is thus irreducible. To see this, ask what the possible subspaces of a 1-dimensional space are.

The case involving degenerate wavefunctions of degeneracy n, where $n > 1$ is more involved, as the representation of these wavefunctions is more complicated (Vvednsky, n.d.). So, we let, $X = \{\psi_1, \psi_2, \dots, \psi_n\}$, be the set of all degenerate wavefunctions associated with some fixed energy eigenvalue E, where $n < \infty$. Moreover, assume X is the smallest set which contains all eigenfunctions and let $V = span(X)$.

We remark that X is a basis by the orthonormality of our wave functions. We will prove any representation of G with representation space V is irreducible via the method of contradiction.

Suppose we have some reducible representation of V. Since V is reducible, we can find some non-trivial subspace W which is stable under the action of G. Consequently, we can find some basis for this subspace, which we call A. We know that:

1. $A \subseteq$ V,
2. Elements in A are eigenfunctions of $\widehat{H}$, since linear combinations of eigenfunctions associated with the same eigenvalue are eigenfunctions
3. $A \neq \emptyset$.

Since W is a subrepresentation and V is reducible, this implies that W is a proper, nontrivial subspace of V. Moreover, since W is invariant under the action of our point group, we know that our matrices given by the representation map elements in W to other elements in W. Thus, we can reduce the set of eigenfunctions of our Hamiltonian to the set A, and thus reduce the degeneracy of our wavefunctions to the set A. Since A is a basis for W, and W is a proper nonzero subspace of V, we conclude that $dim(W) < dim(V)$, which implies $|A| < |X|$. This contradicts the assumption that X was the smallest set which contains all our eigenfunctions (and was thus of

minimal degeneracy). Thus, our representation of these wavefunctions must be irreducible.

Remark: The minimality condition meant we assumed the degeneracy was normal: that is, assuming all our eigenfunctions would be accounted for mathematically (Vvednsky, n.d.). However, experimental evidence might suggest we cannot always account for all degeneracy mathematically. In such cases, the degeneracy is accidental (Vvednsky, n.d.)

3.9 Worked example: H_2O (water)

Let us now, in detail, perform the MO calculations for water (H_2O) using the SALC method. In general, the process has 4 steps:

1. Find the point group of the molecule.
2. Find a representation of the point group (any representation will work)
3. Decompose the representation into irreducibles.
4. Form the MOs by matching atomic orbitals of the same irreducible representations.

Step 3 of this method relies on theorem 12 to ensure we can associate each MO with an irreducible representation and ensure that the set of all the MOs has a representation. From here, the sections regarding characters and irreducible representations ensure we both can break down this representation into irreducibles and provide us with a procedure by which to do so. This section aims to consolidate all the results we collected and show how they can be used in a real-world example.

First, we need to identify the point group of H_2O. This is easiest to do with point group identification flow charts (available on the internet and in many inorganic chemistry textbooks). These make point group identification easier by prompting the reader to identify key conjugacy classes. Using the flow chart given in (Miessler et al., 2022) to identify the point group of water, we get it is C_{2v}.

C_{2v} has 4 elements: $E, C_2, \sigma_v, \sigma_{v'}$, which are the identity, rotation by 180 degrees, and the 2 reflections about the planes highlighted in Figure 2, respectively. These elements are related to each other via the multiplication table below. We include the multiplication table, shown in Figure 4, to be explicit in the description of C_{2v}, but in practice, people just tend to use character tables [more on these later] to pull whatever information they need about the group.

C_{2v}	E	C_2	σ_{v1}	σ_{v2}
E	E	C_2	σ_{v1}	σ_{v2}
C_2	C_2	E	σ_{v2}	σ_{v1}
σ_{v1}	σ_{v1}	σ_{v2}	E	C_2
σ_{v2}	σ_{v2}	σ_{v1}	C_2	E

Figure 4: Group multiplication table for C_{2v}, [obtained from (Pfennig, 2018), Creative Common License]

3.10 Finding a representation of our point group

Having identified our point group, we now seek to find a representation for it. Typically, chemists would find a representation in $\mathbb{R}^3$, but we can observe that our molecule is flat (see Figure 2) since there is a plane on which all 3 atoms lie. Thus, it suffices to find a representation in $\mathbb{R}^2$.

Conventions dictate we orient the molecule, so the origin is where our oxygen is, and the axis of rotational symmetry is the z-axis (Miessler et al., 2022). We placed the molecule on the xz plane, though placing it on the yz plane would make no difference. For each symmetry operation in our group, we aim to find a matrix that has the same corresponding geometric action in $\mathbb{R}^2$ as that group element and compute the corresponding trace. By doing this, we get a representation ρ of C_{2v} in $\mathbb{R}^2$ (Miessler et al., 2022) (Figure 5). Now, we collect traces to obtain the character of each element (Table 1).

$$\rho(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \rho(C_2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \rho(\sigma_{v(xz)}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \rho(\sigma_{v'(yz)}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Figure 5: Representation ρ of C_{2v} in $\mathbb{R}^2$ (Miessler et al., 2022).

Table 1: Reducible representation of water molecule under its point group.

Conjugacy class representative	E	C_2	σ_v	$\sigma_{v'}$
Character of representative	2	0	2	0

Charcters are just maps from a group G to the complex numbers which are constant on conjugacy classes, so this table below is nothing more than a table of values of the character evaluated on all of the group's conjugacy classes. This table gives us a reducible representation of our point group.

Physically speaking, this reducible representation we have obtained does not say much. It just says that the set of all our MOs has these types of symmetries. But this is where the power of decomposing into irreducibles comes in.

By knowing the irreducible representations associated with each atomic orbital, which are easily deduced from character tables, then we know which atomic orbitals interacted to form bonding/antibonding MOs since they must be associated with irreducible representations that have non-zero multiplicity. From this, we know which MO an AO is associated with, since Noether's theorem states that conservation of symmetry is equivalent to conservation of some physical quantity, in this case, angular momentum (Baez, 2020). Thus, atomic orbitals will only overlap to form an MO if they have the same irreducible representations. Knowing the AOs involved in MO formation, we can deduce other MO properties such as energy, spectroscopic properties, and via the dimensionality of an irreducible, degeneracy. To help us decompose our representation into irreducibles, we make use of a character table (Figure 6).

C_{2v}	E	C_2	$\sigma_{v(xz)}$	$\sigma_{v'(yz)}$	Linear functions	Quadratic functions
A_1	1	1	1	1	z	$x^2+y^2+z^2$
A_2	1	1	-1	-1		xy
B_1	1	-1	1	-1	x	xz
B2	1	-1	-1	1	y	yz

Figure 6. Character table for C_{2v}, reproduced from (Kennephol, n.d.) with permission.

We have colour-coded the table for ease of reading, with each section of the table being described as follows (Miessler et al., 2022), (Lowe & Peterson, 2011):

1. Yellow corresponds to the point group.
2. Blue corresponds to the various irreducible representations of our point group, named with respect to the Mulliken symbol conventions (Lowe & Peterson, 2011)
3. Green corresponds to the different conjugacy classes (numbers, if there are any indicate size, and the E, C_n, σ, etc. being representatives. If there are no numbers, assume the number is 1)
4. Purple corresponds to the characters associated with an irreducible
5. Red corresponds to the linear and quadratic rotor functions, which is unimportant for our work

We use the fact that characters on irreducibles form a basis for the characters of all representations. The character table gives us all the information we need about our irreducibles, and Table 1 gives us the characters of our reducible representation we created in step 2. So, we apply the reduction formula to find the multiplicities of each irreducible.

For A_1 , one of the 1-dimensional (irreducible) subrepresentations of C_{2v} in our representation ρ of C_{2v}, we get:

$$m_{A_1} = \langle \chi, \chi_{A_1} \rangle = \frac{1}{|G|} \sum_{i=1}^{k} n_i \overline{\chi_\rho(g_i)} \chi_\rho{}'(g_i)$$

$$= \frac{1}{4}(2 * 1 * 1 + 0 * 1 * 1 + 2 * 1 * 1 + 0 * 1 * 1) = 1$$

Repeating this process with the other irreducibles, we get that $\rho = 1A_1 + 1B_1$. Thus, our MOs have components associated with the A_1 irreducible representation, and another to the B_1 irreducible.

3.12 Matching Atomic Orbitals

Now, we form the MOs from the atomic orbitals we started with, by determining which atomic orbitals interact with each other.

This is where the irreducible representations come in. We first find the irreducible representations associated with each atomic orbital under our point group, done the same way we did it for water. Then, we form the MOs by taking linear combinations of those atomic orbitals that have the same irreducible representation together, so we satisfy Noether's theorem, and by extension the physicists

Now that we know which atomic orbitals make up a given MO, we can form them by adding/subtracting the wavefunctions associated with those atomic orbitals, i.e., taking linear combinations of atomic orbitals. While we could technically take some scalar multiples when we do the LC process, the normalization conditions on wavefunctions make it so there is only 1 value for the scalars. For a set of n atomic orbitals which go on, we should yield n MOs in return, so as to not break physics (which would pose a big problem).

The result of this process yields the following MO diagram below, which has been color-coded. Orange is used to lump the orbitals of type B_1 symmetry, blue to lump those orbitals of type A_1 symmetry, and green to lump those orbitals of type B_2 symmetry. The arrows indicate the electrons that occupy a given MO. We start with the atoms and their orbitals on the edges (before bonding), and the middle has the resulting

MOs which form because of bonding, and we plot everything against their relative energies (**Figure 7**).

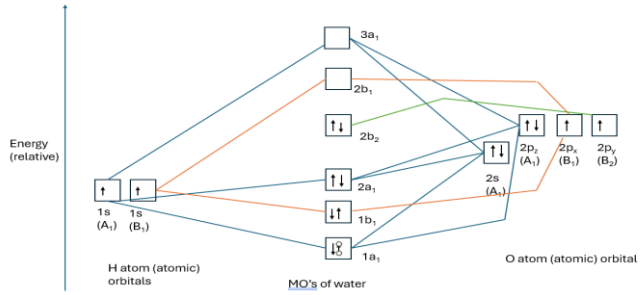

Figure 7: MO diagram for water

Here the energy scale is relative, based on the idea that bonding interactions (adding orbitals) stabilize electrons (and lower their energy), whereas anti-bonding (subtracting orbitals) interactions do the opposite. We use our knowledge of atomic orbitals to guess the extent of bonding/antibonding interactions. Note that we did not use the irreducible representations to assign energies, but merely used them to deduce the atomic orbitals which compose the MO. Only once we knew which AOs formed the MO did we make an educated guess as to their energies.

4 | DISCUSSION

We now aim to see if our mathematical model matches experimental evidence by comparing the predictions made by our MO theory calculations with predictions made by Valance Bond Theory (VBT), a different, but equivalent theory that is also used by chemists (Galbraith et al., 2021). The key difference is that VBT treats electrons as localized entities used to form chemical bonds, whereas MO theory treats them as distributed throughout an entire molecule, with individual wave functions (orbitals) forming the bonds between atoms (Galbraith et al., 2021). Put another way, MO theory treats a molecule as a whole and analyzes the individual parts, whereas VBT uses the parts to analyze the whole. It turns out that both approaches end up becoming equivalent (Galbraith et al., 2021), but both have their advantages and disadvantages.

An important remark here: when we draw Lewis diagrams for any molecule (**Figure 8**), the lines represent bonds, and the dots represent electrons. a pair of electrons is called a lone pair, which is highlighted in blue (Miessler et al., 2022), (Sullivan & Musgrove, 2023).

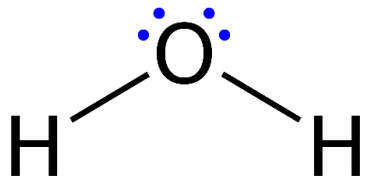

Figure 8: Lewis's structure of Water [Obtained from (*Lewis structure* 2024), Creative Commons license]

When it comes to molecular shape, VBT does seem to do a much better job, because of it is easy to conceptually grasp. Using VBT, one can expect the bond angle between the 2 hydrogen atoms to be approximately $109.5°$ (based on sp^3 hybridization) (Encyclopedia, 2022), whereas the experimental value turns out to be closer to $104.5°$ (Encyclopedia, 2022). VBT attempts to explain this observation by arguing that the lone pair electrons create more repulsion, but a more accurate explanation is given by Bent's rule (Encyclopedia, 2022).

While MO theory can use the shape of water, it involves testing various molecular geometries and finding one that minimizes the total energy (Kennephol, n.d.). This is best done by a computer. Our method is limited in this regard, requiring us to already know what this minimum energy configuration is beforehand. Fortunately, VBT often gets close enough to this minimum for most purposes, and thus acts as a good starting point.

Moreover, this method can only give us information regarding which atomic orbitals combine to form the MO and does not give us the proportion in which they are mixed, which is the physical interpretation of the coefficients in the linear combination. This requires using a computer to solve the Schrodinger equation. However, for rough calculations, this group-theoretic method provides a reasonable approximation.

However, VBT falls short when we consider spectroscopic evidence. VBT would predict that there were 2 bands in a photoelectric spectrum (PES) of water since it assumes both $O-H$ bonds and lone pairs are indistinguishable from each other (Encyclopedia, 2022). However, the PES of water gives 4 different bands, corresponding to energies of 12.6 eV, 14.7 eV, 18.5 eV, and 32.2 eV (Encyclopedia, 2022). Clearly, VBT disagrees with this experimental evidence.

Our group theoretic method produces an MO diagram that contains 4 MOs filled with electrons. These 4 orbitals which have electrons correspond nicely to the 4 bands in the PES of water. More crucially, our method is able to distinguish the energies of the two lone pairs, which VBT cannot.

We can use our MO diagram to correctly make predictions regarding (relative) MO energies for water and by extension the types of reactions water can undergo. For instance, the MO associated with 12.6 eV has high-energy electrons, which are consistent with compounds that are basic. Indeed, water can be seen acting as a base. When H_2SO_4 (sulfuric acid) is mixed with water, we get the following chemical equilibrium (Miessler et al., 2022):

$$H_2SO_4 + H_2O \rightleftharpoons HSO_4^- + H_3O^+$$

Of course, this method relies on our molecule having internal symmetry. Mathematically, this is always possible, since you can always have symmetry by 'doing nothing' and thus have the point group be the trivial one. However, our method really does not work well for molecules that have trivial symmetry, since there is nothing to exploit. However, this method works well for molecules that have non-trivial symmetry.

We were able to show that group theory can play a powerful role in simplifying otherwise complicated calculations involving molecular orbitals. These computations allowed us to make important predictions regarding relative electron energies and can also be used to predict regions of electron density, and thus reactivity on a molecule. However, this model has its limitations, since it only works if there is symmetry to exploit (the point group is non-trivial) and can only predict some molecular properties. Thus, the mathematical model presented in this paper should act as a supplement to more traditional computational methods, and not replace them entirely.

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6 | CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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eureka Research article

The Effects of Avobenzone on the Swim Velocity and Survival Rate of *Danio rerio* Larvae

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ABSTRACT

Background Avobenzone is a UV-A filtering compound found in many personal care products such as sunscreens, cosmetics and soaps. Previous studies found that avobenzone exposure is associated with increased acetylcholinesterase (AChE) activity, which correlates with altered swimming behaviour in aquatic organisms. This study assessed the effects of varying avobenzone concentrations on survival rate and swim velocity in larval zebrafish (*Danio rerio*).

Methods Survival rate was continuously monitored over a 7-day exposure while swim velocity was recorded with behaviour tracking software at 7 days post fertilization.

Results We found that exposure to avobenzone elicited non-monotonic changes to larval zebrafish swim velocity, while leaving the survival rate statistically unaffected.

Conclusions We speculate that avobenzone does not impart high lethality, and that swim velocity changes were caused by energy diversion from locomotor activity to toxicant elimination by active transport at high concentrations.

KEY WORDS: **Avobenzone, Swim velocity, Survival rate, *Danio rerio***

1 | INTRODUCTION

Ultraviolet (UV) filters are chemicals that absorb UV radiation to mitigate sunburns, premature skin aging, and skin cancer (Giokas et al., 2007; Ma et al., 2017; Duis et al., 2022). UV filters can be found in many personal care products, such as sunscreens, cosmetics, soaps, lipsticks, shampoos, and more (Ma et al., 2017). UV-A filters absorb UV light with wavelengths between 320 and 400 nm (Afonso et al., 2014). Upon photon absorption, avobenzone molecules are excited and converted into new compounds called photoproducts that cannot absorb UV light, and therefore, the sunscreen must be reapplied (Afonso et al., 2014). Avobenzone or butyl methoxydibenzoylmethane is present in 71% of sunscreens, making it one of the most common UV-A filters (Bordalo et al., 2022; Afonso et al., 2014).

Avobenzone enters the environment through landfill leachate, wastewater, and direct wash-off from swimmers (Trebše et al., 2016; Duis et al., 2022). Owing to its low molecular weight (310.4 g/mol) and hydrophobicity (log Kow= 4.51), avobenzone has been shown to bioaccumulate and resist biodegradation (Duis et al., 2022). In the environment, avobenzone can be found suspended in sediment, aggregating at the surface of water bodies, and within aquatic organisms (PubChem, n.d.; Liu et al., 2022; Duis et al., 2022). Avobenzone has been found in marine coral, marine mussels, and freshwater fish species at concentrations of 291 μg/kg, 967–7112 μg/kg, and 440–540 μg/kg, respectively (Duis et al., 2022). Additionally, since 1993, personal care product production has increased by an average of 4.5% yearly with a focus on sun protection (Łopaciuk, 2013). The combination of environmental persistence and increased production of avobenzone-containing personal care products highlights the necessity to understand its effects on organism physiology and behavior. This understanding is essential to determining avobenzone's risk to aquatic life and thus its ecological impact.

Previous studies on this issue have found a significant decrease in larval zebrafish locomotor activity with acute exposure (6 days) to avobenzone (Liu et al. 2022). The authors attributed this phenomenon to a significant increase in acetylcholinesterase (AChE) activity induced by

avobenzone. Under normal conditions, AChE degrades the neurotransmitter acetylcholine (ACh), thereby preventing its dispersal and activation of nearby neurons (Trang & Khandar, 2023). Among other processes, voluntary muscle movement is facilitated by ACh (Sam & Bordoni, 2023). Therefore, a decrease of ACh in the neuronal synapse caused by increased AChE can impair muscle contraction.

Previous experimentation has not determined the effect of embryonic exposure to avobenzone. Given that the zebrafish nervous system undergoes rapid differentiation between fertilization and 7 days post fertilization (dpf), exposure to toxicants at this stage can significantly hinder neural cell development and other biological functions (Liu et al., 2022). As a result, our use of swim velocity as an endpoint helps to address whether non-lethal neurological changes caused by toxicants change fundamental organism behaviours (Tierney, 2011).

In the present study, we aimed to test the effects of avobenzone on zebrafish locomotor activity (swim velocity) and monitor changes in zebrafish survival rate. The methodology for this experiment included exposure of zebrafish to increasing concentrations of avobenzone during development. Upon reaching 7 dpf, we assessed the swim velocity of the zebrafish.

We hypothesized that exposing zebrafish to increasing concentrations of avobenzone would decrease swim velocity and survival rates in a dose-dependent manner. We predicted that an increase in AChE may lead to impaired muscle contraction, and therefore, the highest avobenzone exposure concentration (1000 μg/L) should have the lowest swim velocity and survival rate amongst tout of the treatment groups.

2 | METHODS

2.1 Embryo acquisition and maintenance

All procedures complied with the guidelines outlined by the Canadian Council for Animal Care and the University of Alberta. Paired adult wild-type male and female Tupfel-Longfin (TL) zebrafish were placed into spawning tanks 16 hours before embryo collection. Embryos were collected at 1-2 hours post fertilization (hpf). The Petri dishes were maintained at 28.5˚C throughout the experiment.

2.2 Experimental setup

Petri dishes contained 40 mL of E3 embryonic medium (5 mM NaCl, 0.17 mM KCl, 0.33 mM CaCl2, and 0.33 mM MgSO4, pH 7.2–7.4) which provided the necessary nutrients, ions, and pH conditions for optimal embryo growth. Avobenzone solutions contained final concentrations of 10, 50, 100, 500, and 1000 μg/L. In addition, 4 μL of DMSO was added to all Petri dishes to ensure the dissolution of the hydrophobic avobenzone in the water. In our experiment, we introduced an absolute control that contained only the embryonic medium, and a 0.0001 μg/L DMSO solvent control. Each exposure required four successful replicates. A replicate was considered successful if the minimum survival rate for the absolute and DMSO control groups was 70%.

2.3 Avobenzone exposure

Following collection (1-2 hpf), the eggs were placed into the experimental conditions with 60-80 eggs per Petri dish. Daily, 95% of the liquid in each Petri dish was exchanged for fresh embryonic medium, ensuring the maintenance of avobenzone and DMSO concentrations. Deceased embryos were counted, recorded and removed from the Petri dish daily.

2.4 Behavioural assay

At 7 dpf, ten individual larval zebrafish were randomly selected and transferred to the center of a 24 clear-well culture plate. Two culture plates were produced per trial allowing for analysis of 20 fish total. The well plates were placed in a darkroom recording area. Underlighting ensured suitable conditions for recording. After a 20-minute acclimation, the fish were recorded in 5-minute trials. The data was collected and analyzed using EthoVision XT 10 (Nodulus; NE) software for average swim velocity (cm/s).

2.5 Statistical analysis

Initially, we used a single-factor ANOVA to determine if there were significant differences among replicates for the survival rate and swim velocity tests. As no differences were observed, replicates were pooled. We then conducted a Kruskal-Wallis test between the means of all treatment groups for swim velocity. A Kruskal-Wallis test is a non-parametric test that analyzes the variances between means of independent samples with non-normal distributions (McKnight & Najab, 2010). Thereafter, a Tukey HSD Post-Hoc test was conducted to determine the significance of groupings. For survival rate, a single-factor ANOVA test was conducted between the means of all treatment groups. An ANOVA test analyzes the variances between the means of independent samples with normal distributions (McKnight & Najab, 2010). Statistical significance for both tests was accepted at $p<0.05$. All tests were executed using SigmaPlot v15.0.

3 | RESULTS

3.1 Swim Velocity

Overall, there was a significant difference and a non-monotonic relationship between the average swim velocity across treatments (H_6= 37.86, p<0.001) (Figure 1). Average swim velocities for the absolute control, the DMSO control, the 10 µg/L treatment, the 500 µg/L treatment and the 1000 µg/L treatment were 0.051, 0.047, 0.051, 0.064, 0.058, 0.046, and 0.034 cm/s, respectively. According to the Tukey HSD post hoc test, the swim velocity of zebrafish in the 1000 µg/L treatment groups was significantly slower than the absolute control, 50µg/L treatment group, and the 100µg/L treatment group (Table 1). Additionally, the swim velocity at 50 µg/L was significantly faster than the 10, 500, and 1000 µg/L treatment groups (Table 1).

3.2 Survival

In general, there was no significant difference in average survival rate amongst varying avobenzone concentrations ($F_{6,20}$=1.77, p=0.158) (Figure 1). Average survival rates for the absolute control, DMSO control, 10 µg/L treatment, 500 µg/L treatment and 1000 µg/L treatment were 76.4%, 72.3%, 73.1%, 62.1%, 54.0%, 65.8%, 58.2%, respectively. Despite these results being insignificant, there was a general decline in survival rate with increased avobenzone concentration.

4 | DISCUSSION

We hypothesized that if zebrafish embryos are exposed to increasing concentrations of avobenzone, they will display a decrease in swim velocity and survival rate. In this study, we indeed found significant differences in larval zebrafish swim velocity (H_6= 37.86, p<0.001) presenting in a non-monotonic fashion associated with changing concentrations of avobenzone. Zebrafish swimming velocity was initially greater than the control but decreased at high avobenzone concentrations. Additionally, none of our avobenzone concentrations resulted in significant changes to the survival rate ($F_{6,20}$=1.77, p=0.158). However, we did observe a general increase in zebrafish mortality associated with increasing concentrations.

Table 1. Tukey HSD Post-Hoc test determining significance of swim velocity between avobenzone concentration groupings in *Danio rerio* larvae.

Comparison	p-value	Statistically Different	Letter assignment
Absolute control and DMSO	1.000	No	same (a and b)
Absolute control and 10µg/L	1.000	No	same (a)
Absolute control and 50µg/L	1.000	No	same (b)
Absolute control and 100µg/L	1.000	No	same (a and b)
Absolute control and 500µg/L	0.404	No	same (a)
Absolute control and 1000µg/L	<0.001	Yes	different (a/b vs c)
DMSO and 10µg/L	1.000	No	same (a and c)
DMSO and 50µg/L	0.096	No	same (b)
DMSO and 100µg/L	1.000	No	same (a and b)
DMSO and 500µg/L	1.000	No	same (a and c)
DMSO and 1000µg/L	0.105	No	same (c)
10µg/L and 50µg/L	0.049	Yes	different (a/c vs b)
10µg/L and 100µg/L	1.000	No	same (a)
10µg/L and 500µg/L	1.000	No	same (a and c)
10µg/L and 1000µg/L	0.189	No	same (c)
50µg/L and 100µg/L	1.000	No	same (b)
50µg/L and 500µg/L	0.009	Yes	different (b vs a/c)
50µg/L and 1000µg/L	<0.001	Yes	different (b vs c)
100µg/L and 500µg/L	0.902	No	same (a)
100µg/L and 1000µg/L	0.001	Yes	different (a/b vs c)
500µg/L and 1000µg/L	0.648	No	same (c)

Figure 1. The effect of varying avobenzone concentrations on average swim velocity and survival of larval zebrafish. Fish embryos were exposed to treatments from 1-2 hours post-fertilization (hpf) until 7 days post-fertilization (dpf). The absolute control included only embryonic media. The solvent control contained 0.0001 µg/L of DMSO. (A) Kruskal-Wallis statistical analysis was conducted with 4 successful replicates of n=20 to determine significance (H_6= 37.86, p<0.001). (B) Deceased embryos were recorded and removed from the Petri dish daily. Single-factor ANOVA statistical analysis was conducted on 4 successful replicates of n=20 to determine significance ($F_{6, 20}$=1.77, p=0.158). Error bars represent standard error, and the compact letter display shows pairwise-comparisons and significance between treatment groups, where lack of common letters indicates a significant difference in means of the two conditions. Statistical analysis was done in SigmaPlot v15 and the figure was adjusted using Adobe Illustrator.

In accordance with this study, Liu and colleagues (2022) found a significant decrease in zebrafish swim velocity that correlated with increased superoxide dismutase concentrations upon avobenzone exposure. Similarly, a study by Bordalo and colleagues (2022) found significantly higher production of superoxide dismutase in Mediterranean mussels (*Mytilus galloprovincialis)* exposed to avobenzone. Given that superoxide dismutase is a marker for reactive oxygen species (ROS) production, Bordalo and colleagues (2022) suggest that an increase in ROS correlates with an increase in electron transport chain activity. In this case, avobenzone exposure may upregulate cellular respiration to provide the energy needed to eliminate avobenzone from the organism. Decreased swim velocity at high concentrations of avobenzone (1000 µg/L) may have occurred as energy was redirected from locomotor activity to toxicant elimination by active transport (Gupta, 2019). Brewer and colleagues (2001) found similar changes in locomotor activity upon zebrafish exposure to acetylcholinesterase inhibitors diazinon and malathion. They suggested swimming speed is reduced as energy reserves are exhausted.

Both Liu *et al.* (2022) and Bordalo *et al.* (2022) found no significant difference in acute survival rate when the model organisms were exposed to avobenzone at concentrations of 10 µg/L and less. However, Liu and colleagues (2022) propose that avobenzone accumulation in zebrafish over time may lead to chronic toxicity. Taken together, the results of this study suggest that avobenzone exposure does not have significant fatal consequences but may impose sublethal changes to the organism's physiology and behavior.

Limitations of this study include ecological relevance. Environmental concentrations of avobenzone on surface water are much lower than the concentrations used in

our experiments and range from 0.93 ng/L to 2.43 μg/L (Németh et al., 2023). This hinders our ability to imply a direct correlation between our results and what occurs in natural ecosystems. However, low concentrations of a toxicant during a long-term period can elicit similar effects as high concentrations in a short-term study (Van der Eerden, 1982). Furthermore, this study took place in a laboratory setting and thus may not capture the complexities that occur in natural environments (Sabatos-DeVito, 2019).

The broader implications of the results found in this experiment include ecological death. Ecological death occurs when a toxicant impairs an organism's biological functions and imparts sub-lethal consequences, like decreased swim velocity, which eventually indirectly cause death (Scott & Slomann, 2004). Slower fish are unable to easily evade predators or catch prey, ultimately leading to death by predation and starvation (Liu et al., 2022). Decreases in population levels may cause changes in ecosystem dynamics that result in trophic cascades (Lecomte et al., 2009). In worst-case situations, trophic cascades change the population levels of all species in a particular food web and cause irreversible alterations in the ecosystem (Lecomte et al., 2009).

Future studies should examine chronic or multigenerational exposures of avobenzone on zebrafish to explore the bioaccumulation of the compound (Németh et al., 2023). A chronic study could assess the effects of avobenzone exposure after a year at environmentally relevant concentrations to convey chronic morphological and survival rate effects (Liu et al., 2022). Finally, future studies should examine markers to determine the physiological reasons for the decreased swim velocity. Such markers would include AChE quantification and O_2 consumption to measure electron transport chain activity (Shi, 2002).

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6 | CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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eureka Review article

Exploring Empathy and the Right Hemisphere: From Neurological Foundations to Clinical Insights

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ABSTRACT

Empathy, a multifaceted construct encompassing affective responsiveness, cognitive perspective-taking, and emotional regulation, is fundamental to human relationships and societal cohesion. This review examines the right hemisphere's role in mediating empathic processes, drawing upon evidence from neuroimaging, lesion studies, and investigations of gender differences. Findings demonstrate that the right hemisphere is critical for processing emotional cues, such as facial expressions and tone of voice, which are essential for recognizing and responding to others' emotions. Damage to this region significantly impairs emotional recognition and empathetic behaviour, with implications for interpersonal interactions and broader societal dynamics. Furthermore, empathy is not static but evolves throughout life, influenced by biological, cognitive, emotional, and environmental factors. By synthesizing current research, this review highlights the right hemisphere's pivotal role in the neural underpinnings of empathy, providing insights into its developmental trajectory and potential therapeutic targets for enhancing emotional and social functioning.

KEY WORDS: **Right Hemisphere, Neuropsychology, Empathic Functioning, Emotional Processing**

1 | INTRODUCTION

Empathy, the ability to understand and share another person's emotions, is a multifaceted construct involving both affective and cognitive components (Decety & Jackson, 2006). It requires the capacity to experience emotions similar to another's (affective empathy) and the ability to comprehend their thoughts and feelings (cognitive empathy) intellectually (Baron-Cohen & Wheelwright, 2004). While empathy evolves over time and is not a fixed trait, it plays a significant role in fostering compassion, kindness, and altruism in human interactions. Active listening, reflective responding, and perspective-taking enhance empathy by promoting emotional regulation and deeper emotional awareness (Gaspar & Esteves, 2022). Furthermore, empathy is associated with behaviours that reinforce prosocial connections and community bonds, suggesting that empathy is vital not only for individual emotional growth but also for societal cohesion. The right hemisphere of the brain has been shown to play a central role in processing empathy, particularly in recognizing and interpreting emotional cues and adopting another's perspective. Research indicates that the right hemisphere is specialized for processing emotional and social information, with structures like the right frontal lobe, right parietal lobe, and right temporal lobe being particularly involved in these tasks (Davidson & Irwin, 1999; Shamay-Tsoory, 2009). The right frontal lobe, responsible for higher-order cognitive functions, is involved in emotional regulation and decision-making, which are essential for appropriate empathic responses (Miller et al., 2016). The right parietal lobe plays a role in integrating sensory information and understanding social cues, while the right temporal lobe processes auditory and visual information crucial for emotional expression recognition, such as faces and voices (Kosslyn et al., 2014; Schultz, 2016). The occipital lobe, though primarily involved in visual processing, also contributes to the interpretation of emotional expressions (Mishkin & Ungerleider, 1982). Together, these regions enable the brain to process nonverbal communication, which is critical for

recognizing emotions and responding appropriately in social interactions.

Empathy is often classified into three types: cognitive, emotional, and compassionate empathy. Cognitive empathy refers to the ability to understand or infer the thoughts and feelings of others, often tied to the theory of mind (Rueckert & Naybar, 2008). Emotional empathy, in contrast, involves sharing the emotional experiences of others, fostering deeper interpersonal connections (Rueckert & Naybar, 2008). Compassionate empathy, also known as empathic concern, goes beyond understanding and sharing emotions and is coupled with a desire to help alleviate the other person's distress (Goleman, 2006). These types of empathy engage distinct neural pathways in the brain, with cognitive empathy activating the prefrontal cortex, emotional empathy engaging the amygdala and insula, and compassionate empathy requiring an integrative process that activates both cognitive and emotional regions (Shamay-Tsoory, 2009; Decety & Jackson, 2004).

The right hemisphere is particularly important for emotional empathy, with areas like the anterior insula and anterior cingulate cortex being activated in response to the emotional states of others (Decety & Jackson, 2004). Nonverbal communication, such as facial expressions, body language, and tone of voice, plays a significant role in empathy, and the right hemisphere is specialized in processing these nonverbal cues (Davidson & Irwin, 1999). Damage to the right hemisphere can result in difficulties recognizing emotions, understanding social cues, and responding appropriately in social contexts (Adolphs, 2002). For example, individuals with right hemisphere lesions often struggle with tasks involving emotional processing and social interaction. These findings emphasize the importance of the right hemisphere in empathy, highlighting its critical role in interpreting emotional expressions, regulating emotional responses, and facilitating prosocial behaviour. Therefore, empathy is a complex, multidimensional process that involves both cognitive understanding and emotional resonance, with the right hemisphere playing a central role in this process.

2 | NEURAL MECHANISMS OF EMPATHY IN THE RIGHT HEMISPHERE

One of the key players in empathic processing is the anterior insula, which activates when individuals observe others in distress, highlighting its role in emotional empathy. It is integral to the subjective experience of emotions, allowing individuals to resonate with the feelings of others (Craig, 2009). The anterior cingulate cortex also plays a significant role in empathy by integrating emotional and cognitive information, enabling a nuanced understanding and response to others' emotional states. Notably, dysfunction in this area has been linked to challenges in empathic responding, especially in individuals with personality disorders (Keenan et al., 2001).

The mirror neuron system, predominantly located in the right hemisphere, is activated both when a person acts and when they observe someone else performing the same action. This mechanism is believed to underpin the ability to mimic and comprehend the emotions of others, thereby facilitating empathic responses (Rizzolatti & Craighero, 2004). This mirroring effect allows individuals to simulate the emotional experiences of others. Consequently, the right hemisphere's involvement with the mirror neuron system is pivotal in enabling the automatic sharing of emotions, which is central to empathic engagement (Rizzolatti & Sinigaglia, 2010). This is particularly evident when witnessing others in pain or distress, as the same neural circuits are activated as if the observer were experiencing the pain themselves.

Research consistently demonstrates that the right hemisphere is adept at processing and responding to emotional stimuli, with functional magnetic resonance imaging (fMRI) and electroencephalography (EEG) studies showing that it is mainly activated in tasks involving the recognition and interpretation of facial expressions (Lane et al., 1998). Key structures, including the amygdala, insula, and anterior cingulate cortex, are crucial for emotional regulation and empathy (Phan et al., 2002). The right amygdala, in particular, is heavily involved in emotional responses and is particularly sensitive to negative emotions, such as fear or sadness, commonly associated with empathic reactions.

In emotionally charged situations, the amygdala, along with the insula and anterior cingulate cortex, works to modulate the intensity of emotional experiences. Phan et al. (2002) highlighted that these areas, especially within the right hemisphere, are activated when individuals empathize with others' emotional pain. This enables the regulation of both personal and shared emotional experiences, which are fundamental to empathy. Individuals with right hemisphere damage have difficulty interpreting facial expressions, particularly negative emotions (Lane et al., 1998; Decety & Lamm, 2007), emphasizing the hemisphere's role in empathy.

Another essential aspect of empathy involves the regulation of one's emotional responses. Effectively

managing personal emotional reactions while responding to the emotions of others is crucial for healthy social interactions. The right hemisphere, particularly regions such as the anterior cingulate cortex and the prefrontal cortex, plays a vital role in this regulatory process, enabling the modulation of emotional intensity, and assisting individuals in balancing their emotions with those of others (Decety & Lamm, 2007).

When individuals encounter emotionally charged situations, the right hemisphere aids in determining appropriate responses - whether to mirror emotions, as in emotional empathy or to regulate responses to provide support or solutions, as seen in compassionate empathy. The prefrontal cortex is particularly instrumental in managing these complex emotional responses by integrating emotional and cognitive inputs, facilitating a measured and appropriate empathic reaction (Lamm et al., 2011).

The right hemisphere is also crucial for social cognition, encompassing the mental processes that enable individuals to navigate and understand social interactions. Social cognition closely relates to empathy, as it involves the ability to infer the emotions, intentions, and mental states of others, a skill often referred to as theory of mind. Decety and Lamm (2007) found that the right temporoparietal junction plays a significant role in the theory of mind and perspective-taking, both of which are essential for empathic understanding. Damage to this area impairs perspective-taking, reducing empathetic abilities. Moreover, the right prefrontal cortex contributes to moral reasoning and social decision-making, linking empathy to appropriate social behaviours. The ability to understand and predict the thoughts and emotions of others, and to act accordingly, is critical for prosocial behavior, further reinforcing the right hemisphere's integral role in fostering social empathy.

3 | EMPATHY DISORDERS AND RIGHT HEMISPHERE DYSFUNCTION

Individuals with Autism Spectrum Disorder (ASD) often face challenges with empathy and social communication. Neuroimaging studies suggest that altered connectivity in the right hemisphere may contribute to difficulties with emotional recognition and social communication, particularly with social cues (Schultz et al., 2003; Baron-Cohen et al., 2000). Another example of right hemisphere dysfunction is prosopagnosia, a condition characterized by an inability to recognize faces. This often stems from damage to the right hemisphere, impairing empathic engagement as facial recognition is crucial for social interactions (Barton, 2008). Additionally, patients with right hemisphere lesions may struggle with emotional regulation, which can result in inappropriate responses during social interactions, ultimately affecting their relationships and quality of life.

One of the most well-documented effects of right hemisphere damage is the loss or reduction of empathy. Lesions in this region, whether due to stroke, traumatic brain injury, or other neurological conditions, often result in impaired emotional processing and a reduced capacity for empathy. People with right hemisphere damage may have trouble interpreting emotional facial expressions, so they are less responsive to emotional cues and may exhibit flat or inappropriate emotional reactions in social settings. Studies have shown that such individuals also exhibit reduced empathic concern and difficulties with perspective-taking (Shamay-Tsoory et al., 2009).

These findings are consistent with earlier research indicating that the right hemisphere is specialized for processing emotional and social information. Damage to specific areas, such as the temporoparietal junction and the prefrontal cortex, is associated with impaired theory of mind and emotional recognition, both of which are critical for effective empathic functioning (Saxe & Wexler, 2005). Additionally, neurodegenerative diseases that primarily affect the right hemisphere can also result in empathy disorders. Frontotemporal lobar degeneration (FTLD) is one such condition, in which progressive damage to the frontal and temporal lobes, often beginning in the right hemisphere, leads to profound changes in social behaviour. Patients with FTLD frequently experience a reduction in empathy and emotional sensitivity, becoming emotionally detached or indifferent to others' feelings.

The degeneration of structures in the right hemisphere, particularly the orbitofrontal cortex and anterior temporal regions, leads to a diminished ability to empathize with others and a loss of insight into one's own emotions (Gainotti, 2019). Patients with right hemisphere-dominant FTLD often display inappropriate social behaviour, reduced concern for others, and difficulty interpreting emotional signals like facial expressions or tone of voice. The progressive nature of FTLD makes it a key area of study for understanding how right hemisphere dysfunction can result in empathy disorders, as the gradual degeneration of specific brain regions provides insights into the neural basis of

empathy and emotional processing (Rankin et al., 2006). This highlights the right hemisphere's essential role in integrating emotional experiences and supporting social understanding.

Other neuropsychological conditions, such as strokes and tumours in the right hemisphere, also impair emotional regulation and social cognition. Patients with these conditions may experience difficulties with recognizing emotional prosody, leading to misunderstandings in social communication, as people with this damage may struggle to discern whether someone is angry, happy, or sad based on vocal intonation alone. Right hemisphere damage disrupts the ability to interpret emotional expressions, body language, and facial cues, further isolating individuals socially (Adolphs, 2002).

Several psychiatric disorders also involve right hemisphere dysfunction. For example, schizophrenia has been linked to abnormalities in the right hemisphere, particularly in regions responsible for social cognition and emotional processing. Individuals with schizophrenia often exhibit reduced empathy, difficulties in emotional recognition, and impairments in theory of mind (Shenton et al., 2001). These deficits are thought to stem in part from dysfunction in the right temporoparietal junction and prefrontal cortex, areas that are crucial for perspective-taking and emotional regulation.

4 | METHODOLOGICAL APPROACHES TO STUDYING EMPATHY AND THE RIGHT HEMISPHERE

Research on empathy and its neural basis, particularly within the right hemisphere, has been a central area of interest in neuroscience and psychology. Researchers have used various methods—such as neuroimaging, lesion studies, and psychophysiological measures—to explore how the right hemisphere influences emotional processing and empathetic behaviour.

One of the most powerful tools in this research is functional neuroimaging, including functional magnetic resonance imaging (fMRI) and positron emission tomography (PET) scans. These techniques allow scientists to observe brain activity in real time as people engage in tasks that involve empathy. For example, fMRI studies have identified key areas in the right hemisphere, such as the amygdala, insula, and anterior cingulate cortex, which are activated during emotionally charged situations (Phan et al., 2002). These findings have helped us better understand the brain's role in how we process and respond to the emotions of others.

fMRI is also particularly valuable because it tracks changes in blood flow and oxygenation in the brain, providing a non-invasive way to examine brain function. This has proven essential not just for studying empathy in healthy individuals but also for understanding how empathy is affected by brain damage. For instance, research by Shamay-Tsoory et al. (2009) demonstrated that individuals with impairments in empathic concern showed reduced activity in parts of the right hemisphere, particularly areas linked to social cognition, such as the right temporoparietal junction. While PET scans are less commonly used due to their invasive nature and cost, they still offer valuable insights. PET studies often confirm the findings from fMRI by showing reduced metabolic activity in regions such as the anterior insula among individuals with right hemisphere damage, further highlighting the brain's role in emotional empathy (Phan et al., 2002).

Lesion studies, which focus on individuals with localized brain damage, have allowed researchers to compare individuals with right hemisphere damage to those without, revealing significant impairments in emotional recognition, social interaction, and perspective-taking abilities (Shamay-Tsoory et al., 2009). This has been crucial in demonstrating the right hemisphere's involvement in both emotional and cognitive aspects of empathy. For instance, damage to the right prefrontal cortex can lead to significant deficits in empathy and theory of mind, which are critical for understanding others' emotions and making moral decisions (Decety & Lamm, 2007).

Moreover, psychophysiological measures offer further insights into how the right hemisphere governs empathy. These methods include monitoring heart rate variability (HRV), skin conductance, and facial electromyography (EMG) to track emotional and empathic responses at a physiological level. For instance, HRV is often used to assess the balance between the sympathetic (fight or flight) and parasympathetic (rest and digest) nervous systems. Empathic engagement, especially emotional empathy, is linked to increased parasympathetic activity, as shown by higher HRV (Porges, 2001). Studies have also indicated that individuals with right hemisphere damage experience dysregulated autonomic responses, which can interfere with their ability to engage in emotionally attuned interactions.

Skin conductance, which measures the electrical activity of the skin in response to emotional stimuli, has also

been useful in empathy research. Shamay-Tsoory et al. (2009) found that individuals with right hemisphere damage often exhibit weaker skin conductance responses to emotional stimuli, suggesting a diminished physiological engagement with emotional content. Facial EMG, which measures muscle activity associated with emotional expressions like smiling or frowning, has further demonstrated the role of the right hemisphere in generating spontaneous emotional reactions. Research has shown that individuals with right hemisphere damage tend to have asymmetrical facial expressions, with reduced emotion shown on the left side of the face, which is controlled by the right hemisphere (Dimberg & Petterson, 2000).

Behavioural paradigms such as empathy tasks and social simulations are also instrumental in studying empathy. The Empathy for Pain task, where participants observe images of individuals experiencing pain, has shown that people with right hemisphere damage often exhibit reduced emotional responses and lower levels of empathic concern (Lamm et al., 2011). This suggests that the right hemisphere is essential not only for recognizing others' emotions but also for generating appropriate emotional responses to their distress. Role-playing tasks, which require participants to adopt the perspective of another, have similarly demonstrated that individuals with damage to the right hemisphere struggled with perspective-taking, reinforcing the idea that the right hemisphere plays a critical role in cognitive empathy (Shamay-Tsoory et al., 2009).

5 | CONCLUSION

The right hemisphere plays an integral role in shaping empathic experiences. Its involvement in emotional processing, social cognition, and the neural mechanisms underlying empathy underscores the importance of understanding the brain's contributions to empathic behaviour. Insights into the role of the right hemisphere in empathy provide valuable insights into how we can cultivate this essential skill, ultimately promoting healthier relationships and fostering a greater sense of community. Right hemisphere dysfunction, whether due to injury, neurodegenerative disease, or psychiatric disorders, can have profound effects on empathy and emotional processing. The right hemisphere's involvement in recognizing emotional cues, processing nonverbal communication, and engaging in social cognition highlights its critical role in empathic functioning. Damage to this hemisphere can result in significant empathy deficits, as seen in individuals with right hemisphere lesions, frontotemporal lobar degeneration, and other conditions. Continued research on the neural mechanisms of empathy, coupled with the exploration of cultural and social factors, will enhance our understanding of empathy's complexities and its significance in our lives.

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7 | CONFLICTS OF INTEREST

The author declares no conflict of interest.

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Inspiring Change through Curiosity and Innovation

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Dr. Mark Freeman is a Professor of Physics at the University of Alberta and a former Canada Research Chair in Condensed Matter Physics. Beyond his innovative research in nanotechnology and magnetism, he is actively involved in The Shack, a makerspace at the university that empowers students to explore hands-on projects in engineering, design, and technology.

Gopesh Gopinath: Thank you very much for joining me today, Dr. Freeman! We're honoured to have you as our feature researcher for this issue. To begin, could you tell us a bit about yourself, your path to academia, and your connections to the University of Alberta (U of A)?

Mark Freeman: My connection to the U of A is literally lifelong. I was born on campus in the old University Hospital. One of my earliest memories is of my dad, who was a chemistry professor, descending an outside staircase to enter the old physical sciences library – now the site of the undergraduate chemistry labs in the Centennial Centre for Interdisciplinary Science (CCIS). I was about two years old then.

I went on to study physics as an undergraduate at the U of A and attended Cornell University for graduate school. Then, I had an opportunity to stay in New York and work at the IBM Thomas J. Watson Research Center in Yorktown Heights, about 40 minutes north of New York City. At the time, when I went there, it was about as close to an academic environment as you could find outside of a university. I felt like, "This place is amazing. It could be on the dark side of the moon, and I would still want to go there." But things started changing around 1991. After five years at IBM, I started looking for a university post. It wasn't a great time - maybe it never is a great time to look for faculty jobs. But in Canada, big provincial budget cuts were starting in Ontario and Alberta. Somehow, I was extremely lucky to get a job back here and join the faculty.

Was physics always the field that inspired you, or did your interests evolve over time? How did those early experiences shape your commitment to research?

The Apollo moon landing happened when I was nine. I remember sitting on the floor on the veranda at my grandmother's cottage, mesmerized, watching this incredible event unfold. That made a big impression on me and fostered an early interest in astronomy and related fields. After high school, physics seemed to be the science most closely connected to those interests. So I went on to study Honors Physics at the undergraduate level. I even convinced myself that I could pursue physics until I was 40 and then transition to something entirely different – a reflection of youthful optimism.

What kept me in physics, though, was discovering experimentalists – scientists who spent much of their time working in small labs with apparatus they had often built themselves, controlling every aspect of their experiments. The more I learned about that, the more it appealed to me. To this day, it still feels like having a private conversation with nature. Every now and then, nature tells you something new – hopefully something worth sharing with the rest of the world. I also have to give credit to the upper-level

experimental physics courses here at the U of A, as well as a summer job I had at the National Research Council in Ottawa after my second year. Those experiences played a huge role in solidifying my decision to continue with physics after undergrad.

> "To this day, it still feels like having a private conversation with nature. Every now and then, nature tells you something new – hopefully something worth sharing with the rest of the world."

That's fascinating! It's incredible how these seemingly simple experiments can reveal so much about such complex phenomena. Seeing the creativity and precision involved in that process is truly inspiring.

Absolutely! One thing I've found over the years is that, as an experimental physicist, I feel like I've developed a deeper appreciation for some of the amazing things happening in this field. For example, the successful detection of gravitational radiation in 2015 – that was incredible. I'd known about that project in the background for decades, and it always seemed like one of those things that probably wouldn't succeed in your lifetime. It was just so ambitious. I remember feeling such a profound appreciation for what they had accomplished when it happened. In a way, just being able to truly understand and admire that achievement felt like it made all the years of being a physicist worthwhile.

At Eureka, we aim to support undergraduates as they seek out opportunities outside the classroom and grow as researchers. The Shack, another resource here at the U of A, provides hands-on experience that complements classroom learning. Could you tell us about your role with The Shack? What motivated you to help lead this unique resource and how do you see its impact on student innovation and learning?

The traditional physics curriculum is very theory-heavy. It doesn't give the full flavour of what the field is like. When I was a student, I felt pretty lucky to learn more about what physicists did day to day and the variety of activities that encompassed different subfields.

It wasn't until grad school that I fully understood how hands-on physics could be. One of the expectations for experimentalists was to take a shop course, so we could manufacture some of our own custom apparatus for experiments and better design other parts that might require professional machinists to create. I didn't know this was coming, but I discovered I absolutely loved that aspect of experimental physics. It opened up creative outlets for me – you could dream up a part, design it, and then make it to serve a specific purpose.

In doing background reading to draft some of the first proposals for The Shack, I came across a long, fascinating, but not very well-known history of this kind of work. There's an essay called *The Craft of Experimental Physics* by P.M.S. Blackett. He did amazing things during World War II, won the Nobel Prize in 1948, and this essay is part of a 1933 volume called Cambridge University Studies. He described, "The experimental physicist is a Jack-of-All-Trades, a versatile but amateur craftsman. He must blow glass and turn metal, though he could not earn his living as a glass blower, nor ever be classed as a skilled mechanic…The experimental physicist must be enough of a theorist to know what experiments are worth doing and enough of a craftsman to be able to do them." It really resonated with me and captured what it means to be an experimental physicist.

> "It opened up creative outlets for me – you could dream up a part, design it, and then make it to serve a specific purpose."

Now, with the emergence of consumer-oriented 3D printers, it's possible to put the design and manufacturing of custom apparatus into the hands of undergrads. We have a great student shop in our department, and there's a shop course taught by professional machinists, but access for undergrads is limited, and the turnaround times are often impractical for most one-semester courses. With 3D printing, students can dream up a part and have it in their hands the same afternoon. This has made our second and third-year labs much more adaptable. At the same time, The Shack offers tools to others on campus who want to build their own do-it-yourself (DIY) science-related hardware. Over the past 10 years, the U of A has developed a larger ecosystem for innovation, including the Digital Scholarship Centre in the

Cameron Library and the Student Innovation Centre. The Shack is a part of this, and it's been exciting to see how it supports student creativity and learning.

> "Every mistake seems avoidable in hindsight, but perfection isn't realistic in research."

There were a few key developments in late 2013 that helped set the stage. I remember Geoff Steeves from the University of Victoria sent me an email just before Christmas in 2013. It had a picture of a circuit board hanging from a monitor on his desk, running a technical computing platform called Mathematica. That circuit board was one of the first Raspberry Pi® – a $50 board capable of running sophisticated software. Coupled with advances in 3D printing, technologies like this have made it easier and more affordable to introduce programming and computer-interfaced instrumentation into the labs.

A big part of building The Shack has been responding to ideas and enthusiasm from students. It's been incredible to collaborate with so many of them. Ross Lockwood, for example, was one of the first contributors when he was a senior PhD student with Al Meldrum. He was an extraordinary individual with diverse interests – he even competed in a contest to become an astronaut. His office was right across the hall from mine at the time, and I enjoyed exchanging ideas with him. Since then, many others have contributed to the success of The Shack, including Jasmine Mehdwan, Sam Harris, Summer Scott, Robin Robinson, Danielle Jenson, Kayte Mori, Clayton Coutu, Tristan Stark, Logan Fairgrieve-Park, Brian Qi, Adam Cunningham, Grace MacDonald, and Sophie Gans. It's exciting to see undergraduates taking charge and steering The Shack toward new ideas and opportunities.

> "It's often better to focus on a smaller number of things in more depth rather than spreading yourself too thin."

What advice would you give to students looking to take on ambitious, self-directed projects within their undergraduate program, and how do you approach mentorship to support students with diverse goals and interests? What do you think is essential for fostering a strong mentor-mentee relationship in this context?

I think it's important to try and find out if there's something specific students want to get out of a project. Often, it's a general experience, but sometimes there's something more targeted. If that's the case, you can steer things to help them achieve what they're looking for. That said, it shouldn't be about micromanaging the project on their behalf. It's essential to give students enough leeway to make mistakes because, unfortunately, learning from your own mistakes is almost always so much more effective than trying to learn from someone else's. As much as people try to help you avoid repeating their mistakes, it's not the same. It's also important to ensure students don't get lost for too long in blind alleys. High-bandwidth communication is key. The mentor needs to be accessible, and the mentee should keep good project records and regularly share updates.

> "Learning from your own mistakes is almost always so much more effective than trying to learn from someone else's."

For students aiming to pursue ambitious projects, my advice is to seek mentorship early – someone who can give constructive feedback on your proposal and help identify resources to make the project feasible. A common pitfall, even for experienced researchers, is underestimating time. It's easy to misjudge by a factor of ten or more. But once it's approved, we can help arrange access to additional resources, whether that's equipment in The Shack, materials from research labs, or other specialized tools. This collaborative approach fosters creativity while keeping projects manageable.

From what you've observed, it sounds like the most successful students are those who are proactive, open to collaboration, and willing to learn from both their successes and failures. Do you think there's a specific mindset or attitude that helps them stand out in such a dynamic environment?

Curiosity and enthusiasm are the big ones. They naturally lead to motivation to work on a project. Some students might not be as naturally curious or enthusiastic about some of the things happening in courses, but they might find opportunities to engage more in research projects. And, of course, organization and time management are also crucial. Enthusiasm needs to be controlled, and there's some truth in the old saying: if you want to get something done, ask someone who's already busy. Typically, that's someone good at managing their time.

"Recognize the difference between knowing about something and actually knowing it. To really understand something, you have to do it."

I'm going to switch gears a little bit. In the current landscape of open-access research and online learning, students have more avenues for engagement than ever. What opportunities do you think are most valuable for students to explore today, and how can they make the most of the resources available to them?

Absolutely, there's so much out there! I think we're at a point where there's always going to be more and more out there. So, it's crucial to develop a strategy for curating all the available information and honing in on what truly matters. It's often better to focus on a smaller number of things in more depth rather than spreading yourself too thin. In teaching and learning, we talk about this as uncovering a little instead of covering a lot.

"You can't read everything before you start, or you'd never get anything done. Sometimes, you just have to forge ahead."

For me, one influential resource was *Scientific American*. The "Amateur Scientist" column provided interesting do-it-yourself projects. Looking back, I didn't realize at the time how impactful it was, but just reading that column every month was helping to build an interest in me that would eventually find this outlet in experimental physics. Now, of course, there's an overwhelming amount of information available online, but the lesson remains the same: narrowing things down to a smaller selection is key. One approach for filtering through all this is to recognize the difference between knowing about something and actually knowing it. To really understand something, you have to do it. You might see some incredible demos on YouTube, and it only lasts two minutes. But if you're interested in that thing, it might be worth trying to recreate it yourself. When you do, you'll undoubtedly discover there are so many more layers to it that didn't come through in the video. This is a crucial step in curating and winnowing down the vast amount of knowledge out there, and it's a strategy that can guide students in their research and learning.

The path of scientific research often comes with challenges, and resilience is key. Could you share a time in your career when you faced a setback or challenge? How did you overcome it, and what did it teach you about persistence in research?

One thing that has always stuck with me is a saying of one of my professors. He said, "The second one is always better." The idea is that when things go wrong, you should take it in stride and try again. During my PhD work, I needed to vacuum anneal a copper piece that had to remain vertical during the process because copper softens at annealing temperatures, and it would collapse if positioned sideways. Unfortunately, the furnaces in the department were all horizontal tube furnaces, so I had to design and build a vertical tube furnace myself. I found a stainless steel tube in the shop that seemed perfect for the vacuum chamber. What I didn't realize was that when the steel got hot under a vacuum, it became soft and collapsed during the annealing process. I later learned this collapse pattern is a well-documented phenomenon, forming a distinctive threefold pattern around the circumference of the tube. If I had done more research beforehand, I might have anticipated this issue – but that's part of the trade-off in research. You can't read everything before you start, or you'd never get anything done. Sometimes, you just have to forge ahead. Ultimately, I managed to cut my part free from the collapsed structure, procure a quartz tube, and upgrade the furnace to continue my work. That experience reinforced an important lesson: every mistake seems avoidable in hindsight, but perfection isn't realistic in research.

On the other hand, could you share a memorable breakthrough or a 'eureka' moment that stands out in your career?

I've always really enjoyed building new experiments – almost as much as actually running them. I find it so rewarding to dream up a new way of studying something, design the apparatus, and then see it all come together. For me, the emphasis has been more on the journey than the destination.

One example that stands out is from my time at IBM. We were developing a new way to study dynamics in magnetic microstructures. Essentially, we figured out how to make stroboscopic movies of these dynamics, combining optical microscopy with short-pulse lasers as the light source. By analyzing the polarization of the reflected light, we could extract magnetic information in what's called "time domain measurements." This allowed us to capture snapshots of dynamics happening on the scale of picoseconds. Before this, most studies of magnetization dynamics were done in the frequency domain using radio or microwaves, which lacked the spatial resolution you can get with optical microscopy. While the frequency and time domain approach are mathematically linked through Fourier transforms, the addition of spatial resolution made a huge difference. Some specialists at the time initially doubted that we could do what we claimed. But having both spatial and time information together made it much easier to compare experimental results with theoretical models of this physics, which naturally work across both domains. It was a lot of fun, and it felt like we were pushing the boundaries of what was possible.

> "Really get to know yourself! Be sure that the goals you're pursuing are genuinely your own, and not what others think you should be chasing."

Looking back, is there any advice you would give to your undergraduate self, knowing what you do now about the journey through academia? Is there anything you wish you'd known or done differently?

I'm sure you've heard this: "Always do your best, and anything worth doing is worth doing well." I heard that a lot and I tried to live by it. But there's a caveat to this advice. Your best depends on the context. In most cases, you're doing your best within the time available. You can't always do your absolute best for everything because time is often limited. So, in those situations, your best is whatever you can do within the time constraints. The moments that truly require your absolute best are few and far between, and when those come up, you need to make the time and space to give it everything you've got. But most of the time, that's not possible. This is something I wish I'd known sooner as it would have alleviated a lot of stress in many situations.

Also, when you dive deep into research, you often think you've discovered something totally new, only to find out that someone, decades ago, had the same idea – or something similar. Maybe they didn't have the same technology at the time, but it just reinforces the idea that there's nothing new under the sun. It's all about perspective. Things may seem to change fast at a micro level – like the new equipment in the lab, the shift from analog to digital technology, or even the new administrative procedures we have to follow. But on a broader, longer timescale, a lot of these changes are just refinements of what came before. For example, even though lasers today can do things unimaginable back in the '80s, they still existed before. It's the details that change over time, and it's important to keep that perspective in mind.

Looking ahead, with all the uncertainty around AI, climate change, and other global issues, I feel that 50 or 100 years from now, people will still look back and think, there's nothing new under the sun. All of these massive upheavals, as they seem in the moment, will eventually be seen as part of a much larger continuum.

> "Explore broadly and let the satisfaction of the work guide you, rather than feeling locked into one particular direction."

That's such an important point you made about balancing the drive to give your absolute best with being kind to yourself. Lastly, for undergraduates who might be uncertain about their direction in science, what advice would you give? How can they balance the need for exploration with the pressures

of career planning, and are there paths that are often overlooked but worth considering?

Firstly, really get to know yourself! be sure that the goals you're pursuing are genuinely your own, and not what others think you should be chasing. University students, especially, can often feel the weight of expectations from others, but those shouldn't be the foundation of your career choices. Focus on identifying what truly excites you – whether it's solving problems, creating things, or learning new concepts. Research problems, as we know, tend to be hyper-specific, but the satisfaction from solving them is more universal. I love puzzles, so research is a great fit because it's all about tackling puzzles. But the specific puzzle doesn't matter as much as the process of diving into it and figuring it out.

It's also helpful to adopt a broad perspective. In any job, especially in science, satisfaction often comes from what you bring to the table, not just what the job demands from you. That's why it's important not to be too rigid or overly specific in your career goals. So, my advice is not to feel pressured into finding a super specific path right away. Explore broadly and let the satisfaction of the work guide you, rather than feeling locked into one particular direction.

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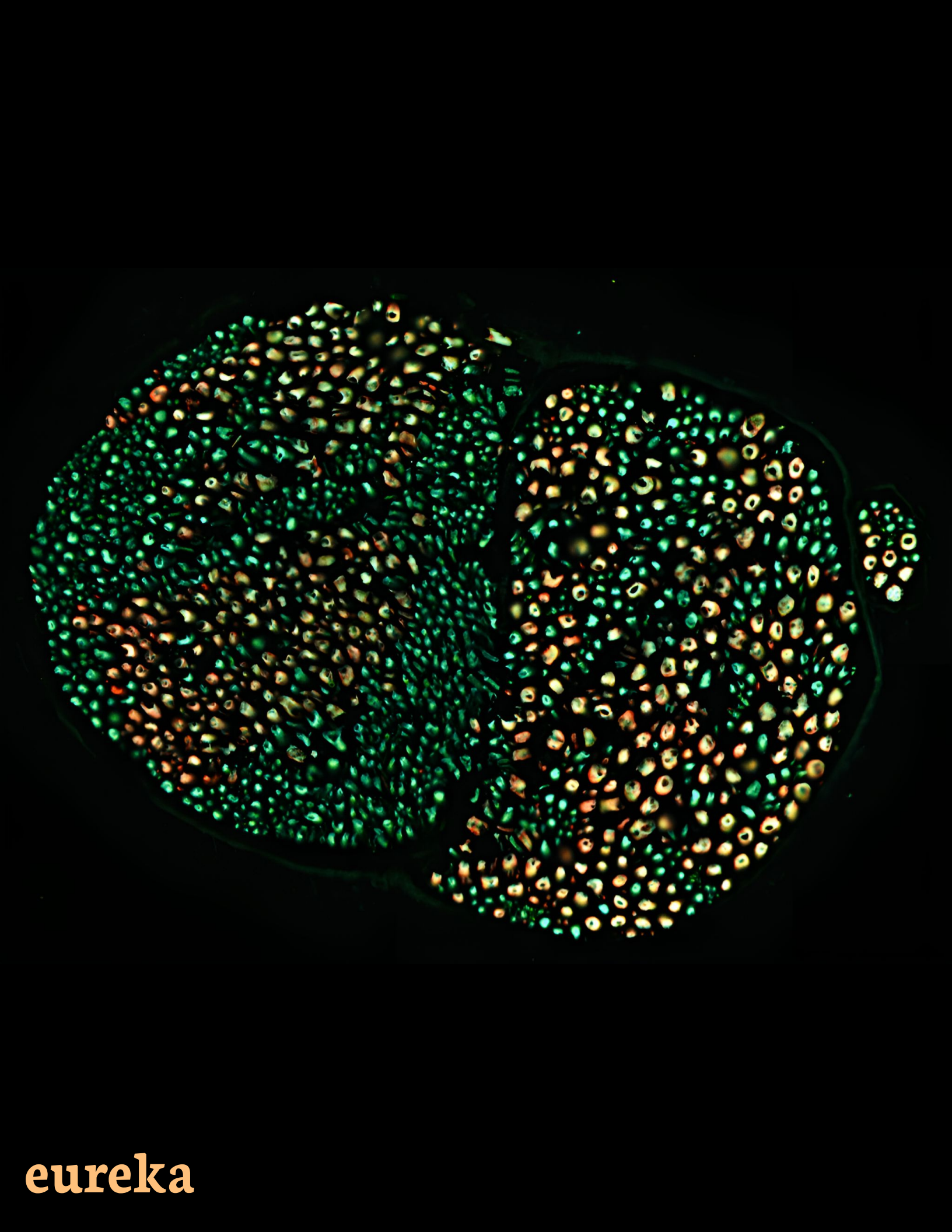

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