



Rutgers-NASA Annual ENIGMA Astrobiology Symposium

ENIGMA: Evolution of Nanomachines In Geospheres and Microbial Ancestors

How did proteins evolve to become the predominant catalysts of life on Earth?

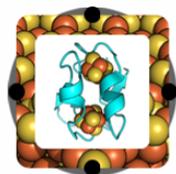
May 10-11, 2022

Tuesday 9:00am-5:00pm EDT

Wednesday 9:00am-3:00pm EDT

Virtual symposium to inform astrobiological research and help us to better understand the origins and evolution of life.

enigma.rutgers.edu

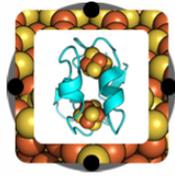


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Evolution of Nanomachines In Geospheres and Microbial Ancestors

Day 1 - May 10th

Time - EDT	Speaker	Title
9:00am-9:10am	Paul G. Falkowski, PI ENIGMA, Rutgers University	Welcome and Introduction
9:10am-9:30am	Vikas Nanda, Co-PI ENIGMA, Rutgers University	Theme 1 Overview
9:30am-10:15am	Salma Kassem, City University of New York	Approaches for the in-situ emergence of functionality in peptide-based systems
10:15am-10:30am	Break	
10:30am-10:50am	Yana Bromberg, Co-PI ENIGMA, Rutgers University	Theme 2 Overview
10:50am-11:35am	Nir Ben-Tal, Tel Aviv University	Protein archeology: How proteins emerged and evolve?
11:35am-12:00pm	Nathan Yee, Co-PI ENIGMA, Rutgers University	Theme 3 Overview
12:00pm-1:00pm	Lunch	
1:00pm-1:25pm	Dru Myerscough, Rice University	Determinants of multiheme cytochrome electron transfer uncovered by systematic mutation
1:25pm-1:50pm	Bhanu Jagilinki, Washington State University	Selenium oxidoreductases - a promising alternative biochemistry for more reducing worlds
1:50pm-2:15pm	Kenneth McGuinness, Rutgers University	Expanding ENIGMA's 1) public exposure and 2) modeling space
2:15pm-2:40pm	Saroj Poudel, Quantum Si	Ecological distribution of nitrogenase reveals modern isoforms evolved to potentially bind charged proteins to mitigate oxygen toxicity
2:40pm-3:05pm	Diego Ferreira, University Buenos Aires	From evolution to folding of repeat-proteins
3:05pm-3:20pm	Break	
3:20pm-3:45pm	Anirudh Prabhu, Carnegie Institute for Science	Can network science help identify biosignatures?
3:45pm-4:30pm	Akif Tezcan, University of California San Diego	What does it take to fix nitrogen?
4:30pm-5:00pm	Open Discussion	



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Evolution of Nanomachines In Geospheres and Microbial Ancestors

Team Leaders



Paul G. Falkowski
Rutgers, Distinguished Professor, PI ENIGMA Program
Bennet L. Smith Endowed Chair



Vikas Nanda
Theme 1
Rutgers, Professor
Ctr. for Advanced Biotechnology and Medicine



Yana Bromberg
Theme 2
Rutgers, Professor
Dept. of Biochememistry
and Microbiology



Nathan Yee
Theme 3
Rutgers, Professor
Dept. of Environmental Sciences



Shaunna Morrison
Theme 3
Carnegie Institute for Sciences
Carnegie Research Scientist
Earth and Planets Laboratory



Robert M. Hazen
Theme 3
Carnegie Institute for Sciences, Senior Staff Scientist
Earth and Planets and Geophysical Laboratory



Janice McDonnell
Education and Outreach
Rutgers, Associate Professor
4-H Science Engineering Technology (SET) Agent

Speakers



Salma Kassem

Salma Kassem obtained her PhD from the University of Manchester (UK) working on bio-inspired molecular machines. She joined the group of Prof. Ulijn in 2019 at CUNY ASRC to work on new approaches for the discovery of functional peptide based systems. Salma is interested in bridging the gap between artificial molecular machines and peptide nanotechnology.

Abstract: Approaches for the in-situ emergence of functionality in peptide-based systems. The emergence of life from simple building blocks is an intriguing and mysterious subject of research and constant discussion. The functionality of living systems is, in big part, derived from the assembly and interaction of the 20 gene encoded amino-acids that make up proteins. Our work focuses on understanding the rules that govern self-organization and compartmentalization of amino-acids, by developing biomimetic approaches using short peptides. We explore the complexity of systems that arise from dynamic combinatorial peptide libraries and the compartmentalization of functional structures in condensates. By focusing on the design and discovery of new modalities rather than adaptation or simplification of known biological systems, we also gain insights into design concepts for repurposing life's building blocks beyond the biological context.



Nir Ben-Tal

Nir Ben-Tal is a full professor in the Department of Biochemistry and Molecular Biology, George S. Wise Faculty of Life Sciences, Tel Aviv University.

Ben-Tal completed his bachelor degree in Biology, Chemistry and Physics at the Hebrew University of Jerusalem, Israel, in 1988, and his DSc in Chemistry at the Technion, Israel Institute of Technology, in 1993. Later he did his postdoctoral training in biophysical chemistry at Columbia University, New York. In 1997 Ben-Tal accepted a faculty position at the department of Biochemistry and Molecular Biology, Tel Aviv University, and became full professor in 2007.

The Ben-Tal lab studies the general area of computational structural biology. The work includes both methodology development and applications to selected problems. They have been developing the ConSurf methodology and web-server for the detection of interaction regions in proteins based on evolutionary data (<http://consurf.tau.ac.il/>), as well as tools for searching and navigating in protein space

Abstract: Protein archeology: How proteins emerged and evolve? Since their emergence about 3.7 billion years ago, proteins have been key to life as we know it. But how did they emerge and continue to evolve? The straightforward path, involving the addition of one amino acid after another—starting from scratch, is bound to fail, as the vast majority of such arbitrary strings can't even form stable structures, let alone function. Therefore, instead, evolution follows a cut-and-paste approach, where amino acid segments from existing proteins are grafted and stitched together to form new proteins. We know this, because the latter approach leaves traces, in the form of reused segments. By tracing these, we aim to decipher the origin of proteins, similarly to archeologists tracing human history.



Dru Myerscough

Dru Myerscough

Undergraduate - Major Biochemistry, Minor Cell Biology
Rice University

Abstract: Determinants of multiheme cytochrome electron transfer uncovered by systematic mutation. Cellular assays are a versatile strategy to study electron transfer mediated by protein electron carriers, including ferredoxins, flavodoxins, and cytochromes. To investigate sequence-structure-function relationships in multiheme cytochromes, we used *Shewanella oneidensis* respiration on Fe(III) as an assay for electron transfer mediated by MtrA, a multiheme cytochrome that resides within the outer membrane porin MtrB. In this talk, we will describe our efforts to develop a growth selection for MtrA, generate an MtrA mutant library, and select for variants that support the reduction of extracellular materials. We will also discuss our efforts to evaluate how mutations affect cellular reduction of extracellular materials, and we will reflect on how mutation tolerance relates to functional motifs and coordination of heme cofactors.



Bhanu Jagilinki

Bhanu Jagilinki is currently a post-doctoral researcher at Washington State University.

Dr. Jagilinki received his PhD in India at the Advanced Centre for Treatment, Research and Education in Cancer, Navi Mumbai, and then moved to the MIGAL Galilee Research Institute in Israel, where he was introduced to metalloproteins. He was fascinated by how metalloproteins carry out so many complex biological reactions by simply modulating its redox states. His passion towards metalloproteins brought him to Rutgers University, where he worked with mini-ferredoxins believed to be predecessors for the modern metallo-enzymes. To further explore the molecular mechanisms behind the catalysis, Jagilinki joined Peters lab at WSU to understand the catalytic bias in the natural hydrogenases.

Abstract: Selenium oxidoreductases - a promising alternative biochemistry for more reducing worlds. Selenium is an essential trace element in many species including humans, however not universal to all living organisms. There are several selenium containing proteins (selenoproteins), most of them involved in catalyzing chemical reactions or maintaining redox homeostasis. These enzymes have selenocysteine (Sec) in their sequences, which is very similar to cysteine (Cys) where thiol group is replaced by a selenol. In sulfur-containing enzymes, substitution with selenium generally does not impact function. However, the reverse is not true and will completely abolish the enzymatic activity. We have selected two minimal ancestral ferredoxins which upon chemical reconstitutions with Fe and Se salts, assembles with two [4Fe-4Se] clusters. In comparison to the counterparts coupled to [4Fe-4S], the ancestral mini-ferredoxins with [4Fe-4Se] clusters have lower mid-point potentials. Se-containing protein electron carriers would provide an advantage in more reducing environments. Also, our thermotical calculations under more reducing and lower pH conditions, Se was found to be more stable than sulfur. A selenium-based alternative biochemistry might exist on other worlds. Future orbital and lander explorations of more reducing worlds with higher selenium content, could consolidate this hypothesis.



Kenneth McGuinness

Kenneth McGuinness is an ENIGMA Post-doctoral Researcher at Rutgers University. Raised a Jersey boy - studied at Rutgers - enjoyed time in industry - heart is sparked by teaching scientific thinking.

Abstract: Expanding ENIGMA's 1) public exposure and 2) modeling space. Quick question: 1) How do we increase ENIGMA's exposure to the public? Could it be a new YouTube channel dedicated to interviews with the ENIGMA team members? In particular, ENIGMA authors? Join me for a thrilling interview with our very own Professor Yana Bromberg and RISE graduate, Falade Aderibigbe, as they have a conversation about recent findings that lead to break throughs on how to better understand protein evolution. 2) Molecular dynamics is an incredible tool for understanding proteins atomically. Come join me as I describe the use of molecular dynamics in understanding the mechanism of how organic material (i.e., amino acids) adsorb and interact atomically with mineral surfaces (i.e., brucite) thought to be an important player in the hydrothermal vent theory of how life may have originated.



Saroj Poudel

Saroj Poudel is currently a Senior Bioinformatics Scientist at Quantum Si. He combines both his sequence and structural computational skills to analyze and design proteins essential for next generation sequencing.

Abstract: Ecological distribution of nitrogenase reveals modern isoforms evolved to potentially bind charged proteins to mitigate oxygen toxicity.

Nitrogenase catalyzes the reduction of dinitrogen gas to bioavailable ammonia. Though it emerged only once, it has evolved across both bacterial and archaeal domains and, increasing evidence suggests, across the globe. To better understand the evolutionary path of nitrogenase, we investigated its geographic and phylogenetic distribution and the structural dissimilarities that might account for their diversity. We identified >850 novel nitrogenases of which most were abundant in subsurface environments (e.g., deep sediments) but present across a wide range of surface environments (e.g., surface waters). Higher cophenetic distances of identified homologs suggest a higher evolutionary rate for molybdenum-containing isoforms (Nif) than their other types. Structural analysis of the Nif isoform revealed a charged pocket in the homodimeric iron protein that could host an oxygen tolerant substrate protecting it from oxidative stress. Together, our study revealed a greater diversity of nitrogenase isoforms in new environments and a mechanism to mitigate oxygen toxicity.



Diego Ferreiro

Diego Ferreiro is an Adjunct Professor in the Department of Biological Chemistry at the Universidad de Buenos Aires, Argentina. Originally trained as a Biologist, Diego did a PhD in Biochemistry at the Univ. Buenos Aires and postdoc in Biophysics of protein folding and function at UCSD. Since 2010, Diego co-directs the Protein Physiology Laboratory in the Biological Chemistry Department at Univ. Buenos Aires, investigating the relations between sequences, structures, dynamics and evolution of protein molecules.

Abstract: From evolution to folding of repeat-proteins. Protein sequences change by a multiplicity of evolutionary mechanisms. Fixation of these changes is coupled to the protein's capability to properly explore the conformational space and perform biological functions. Repeat-proteins are privileged systems to understand the relations between evolution and folding, due to their symmetries and functional diversity. Here, we interpret the evolutionary record in natural sequences to model and analyze the folding mechanisms of thousands of proteins. The proposed model successfully reproduces folding experiments using only sequence information as input. We further perform large scale predictions of folding mechanisms in the most abundant repeat-protein family, identifying higher order features such as domain emergence, stability, and cooperativity of repeat-arrays.



Anirudh Prabhu

Anirudh Prabhu is a Geo-informatics Scientist at the Earth and Planets Laboratory in the Carnegie Institution for Science. Prabhu holds a PhD in Multidisciplinary Science from RPI. During his PhD, Prabhu worked at Tetherless World Constellation and was advised by Prof. Peter Fox and Prof. Deborah McGuinness.

Prabhu's research involves developing algorithms, visualizations, and methods in the fields of Artificial Intelligence, Machine Learning and Informatics and their application in a variety of domains such as Earth and Space Science, Paleobiology, and Microbiology. The path to achieving this goal lies in a truly multidisciplinary approach, harnessing the integrated power of multiple scientific domains by using data as the backbone of the discovery process. This in turn required solving problems that plague the fields of data science, knowledge extraction, and data visualization, for example, how to deal with extremely small or sparse data, how to extract the relationships embedded in unstructured text, how to deal with scalability issues with extreme large number of attributes for data mining algorithms, such as affinity analysis.

Prabhu was the Student Representative of the Geo-informatics and Data Science Division of the Geological Society of America from 2018 to 2021, and has been a member of the Data Science Team of both the [Deep Carbon Observatory](#) and the [4D initiative](#) since 2016. Prabhu was also awarded the IBM Global Fellow Initiative in 2015. Prabhu was a collaborator on the NASA MSFC DarkData Project from 2014 to 2017. Prabhu has been awarded the "Founder's Award of Excellence" at RPI.

Abstract: Can network science help identify biosignatures? Network science is an academic field which studies complex enviro considering distinct elements or actors represented by nodes and the connections between the elements or actors as edges. Using networks can help view existing chemical, geological and biological information systems from a purely mathematical perspective, and infer new relationships or new information about existing relationships. In this talk, we'll focus on some new and exciting explorations to see if we can identify potential biosignatures through network analysis. We will highlight two very nascent projects where we: 1) Analyze planetary atmospheric networks to identify potential for life in planets based on the chemical composition of their atmospheres and 2) Using network science to distinguish biotic and abiotic GCMS (Gas Chromatography Mass Spectrometry) samples.

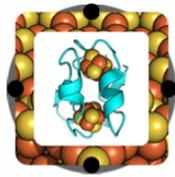


Akif Tezcan

Akif Tezcan is a Professor and Leslie Orgel Faculty Scholar in the Department of Chemistry and Biochemistry at the University of California, San Diego.

Dr. Tezcan is also a faculty affiliate in the Department of Nanoengineering and a member of the Materials Science and Engineering (MSE) Program and the Institute of Materials Discovery and Design at UCSD. Tezcan was born and raised in Istanbul, Turkey, received his BA (chemistry/biology) at Macalester College (St. Paul, MN) and completed his PhD and postdoctoral studies at Caltech (Pasadena, CA) with Harry Gray and Doug Rees, respectively. Tezcan is a bioinorganic and biophysical chemist by training. His research program, started at UCSD in 2005, focuses on developing new chemical tools and strategies to study biological nitrogen fixation, to design functional proteins and enzymes, and to create new biomaterials.

Abstract: What does it take to fix nitrogen? Reduced forms of nitrogen are essential for the biosynthesis of amino- and nucleic acids. As the only enzyme capable of nitrogen fixation, nitrogenase catalyzes the eight-electron reduction of atmospheric nitrogen and protons into ammonia and hydrogen. Nitrogenase is distinct from most redox enzymes in its requirement for adenosine triphosphate (ATP) hydrolysis to enable the successive transfer of electrons and protons for substrate reduction. Yet, despite decades of extensive research, it is not understood 1) why/how ATP hydrolysis is used to “power” nitrogen reduction and 2) how the catalytic reaction proceeds. In this presentation, I will present our recent experimental/structural findings that begin to shed light on these questions.



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Evolution of Nanomachines In Geospheres and Microbial Ancestors

Day 2 - May 11th

Time - EDT	Speaker	Title
9:00am-9:05am	Paul G. Falkowski, PI ENIGMA, Rutgers University	Welcome and Introduction
9:05am-9:55am	Michael Wong, Carnegie Institute for Science	From NOx to Networks: My astrobiological journey
9:55am-10:20am	Shaunna Morrison, Carnegie Institute for Science	A brief introduction to the mineralogy of Mars
10:20am-10:45am	Corday Selden, Rutgers University	Experimental investigation of amino acid binding as a mechanism for fractionating metal stable isotopes in proteins
10:45am-11:00am	Break	
11:00am-11:45am	Daniel Hummer, Southern Illinois University	Data Mining the Past: Using large mineral datasets to trace Earth's geochemical history
11:45am-12:00pm	Janice McDonnell, Rutgers University	Education and Outreach Overview
12:00pm-1:00pm	Lunch	
1:00pm-1:45pm	Kevin Hand, NASA Jet Propulsion Laboratory	Alien Oceans: The search for life in the depths of Space
1:45pm-2:30pm	Open Discussion	



Michael L. Wong

Michael L. Wong is a Carnegie Postdoctoral Fellow at the Carnegie Institution for Science's Earth & Planets Laboratory studying planetary atmospheres, habitability, biosignatures, and the emergence of life. In his spare time, he hosts a podcast called Strange New Worlds, which examines science, technology, and culture through the lens of Star Trek.

Abstract: From NO_x to Networks: My Astrobiological Journey. Life is a quintessential far-from-equilibrium system that harnesses external disequilibria to perform its functions. In one hypothesis for life's origins, redox and electrochemical disequilibria inherent to submarine alkaline hydrothermal vents could have provided the driving force for the onset of metabolism. One critical component of this framework are nitrogen oxides, which would have provided a high-potential electron acceptor as well as a source of fixed nitrogen to nascent biological systems during the Hadean. We simulate the production of nitrogen oxides in Earth's early atmosphere by using a novel combination of a general circulation modeling and photochemical modeling. Applying this modeling framework to early Mars reproduces the concentration of nitrates found in the mudstones of Gale Crater to within a factor of ~2. Life is also a quintessential evolving system in which information plays a principle organizing role, structuring flows of free energy and matter. In ongoing work, we are investigating whether (and how) it may be possible to distinguish living from non-living worlds through the metrics of their atmospheric chemical networks.



Shaunna M. Morrison

Shaunna M. Morrison is a mineralogist and planetary scientist with expertise in crystallography, crystal chemistry, and the application of data driven techniques.

Morrison is the 4D (Deep Time Data Driven Discovery) Initiative Co-Director at the Carnegie Institution for Science's Earth and Planets Laboratory, former Project Manager of the Carnegie led Deep-Time Data Infrastructure (DTDI), a Co-Investigator of the CheMin X-ray diffraction instrument on the NASA Mars Science Laboratory (MSL) mission, a collaborator on the NASA Astrobiology ENIGMA Project, a Co-Investigator of the NASA Astromaterials Data System, and a data contributor and collaborator of the RRUFF Project, including the Mineral Evolution Database (MED), Mineral Properties Database (MPD), and the Evolutionary System of Mineralogy Database (ESMD). Morrison builds on her technical and theoretical background in crystallography, crystal chemistry, and martian mineralogy, to explore new techniques in multidimensional, multivariate analysis and visualization by employing a range of advanced analytics and machine learning techniques to better understand the complex relationships among Earth and planetary materials, their formational environments through deep time, and their coevolution with the biosphere.

Abstract: A brief introduction to the mineralogy of Mars. As one of our nearest neighbors and an analog for early Earth, Mars has been the subject of much study, including remote sensing and surface missions, with sample-return missions currently in the works, and extensive study of martian meteorites. In this presentation, we will introduce the methods by which we determine mineralogy on Mars, the mineralogical and geochemical data that are currently available on these materials, and new martian meteorite mineral networks. The discussion of our newly compiled database of martian meteorite minerals and its associated networks will include a comparison of the similarities and differences between what we observe in martian mineral networks versus that of Earth's minerals and an outline of the underlying causes of the divergence related to planetary evolution.



Corday Selden

Corday Selden is an ENIGMA Post-doctoral Researcher at Rutgers University.

Selden is a biogeochemist with expertise in stable isotope geochemistry and molecular biology. Her work centers on the reciprocal dynamics between microbes and their physico-chemical environment, how these dynamics shape the Earth system, and the imprints they impart. Currently, Corday is exploring the mechanisms which underpin biological fractionation of stable metal isotopes (e.g., Cu, Zn, Ni). This work is pivotal to developing metal isotopes as tools for tracking microbial metabolism in modern and ancient environments.

Abstract: Experimental investigation of amino acid binding as a mechanism for fractionating metal stable isotopes in proteins. Cellular metabolism depends on transition metals as protein co factors. As cellular activity partitions metal isotopes, their ratios can be used to trace biological function. Ab initio calculations suggest that the incorporation of transition metals into proteins can impart an isotopic fractionation dependent on the metal binding site and, particularly, on the identity of the coordinating amino acid ligands. We investigated the isotopic fractionation of zinc and copper due to coordination by amino acids common at protein metal-binding sites. The objective of this study was to constrain equilibrium isotope fractionation values for amino acid-bound metals. Sulfur- and nitrogen-bearing ligands were found to impart inverse isotope effects. This work adds to the growing body of evidence that metalloprotein biosynthesis can affect the distribution of transition metal isotopes in biological systems.



Daniel Hummer

Daniel Hummer is an Assistant Professor of Geology at Southern Illinois University in Carbondale, Illinois. He is a mineralogist and geochemist whose research attempts to answer fundamental questions about how minerals crystallize, how crystal structure dynamics result in different phase stabilities, and how Earth's mineralogy has changed over time.

Hummer received B.S. degrees in both Geology and Chemistry from Iowa State University in 2004, and a Ph.D. in Geoscience from Penn State University in 2010 working on aqueous crystallization of titanium oxides. Subsequently, he was a postdoctoral researcher at the Carnegie Institution for Science and UCLA before starting as an Assistant Professor at Southern Illinois University in 2016. Hummer has earned multiple awards for his work in experimental mineralogy, including a fellowship at the Carnegie Institution for Science, and the Kraus Award for Crystallographic Research from the Mineralogical Society of America.

Abstract: Data Mining the Past: Using large mineral datasets to trace Earth's geochemical history. Changes in redox state between the crust, mantle, and atmosphere are critical to understanding Earth's evolution, but these changes are difficult to correlate on global scales. Techniques leveraging large data sets can illuminate geochemical changes across large temporal and spatial scales. In particular, manganese is a redox-sensitive metal whose abundance in crustal minerals makes it a useful tracer of crustal oxidation. Analysis of global Mn mineral occurrences shows that the oxidation state of crustal Mn has risen during the Phanerozoic in direct response to atmospheric oxygenation. Recent work in the Hummer group on the evolution of Cu and Fe-bearing minerals also demonstrates that large data sets of redox sensitive mineral systems can constrain the evolving redox states and interactions of various Earth reservoirs.



Janice McDonnell

Janice McDonnell is currently serving as the Science Engineering & Technology Agent for the department of 4-H Youth Development at Rutgers University where she supports county 4-H Agents in promoting STEM in their communities.

McDonnell hosts a variety of on-campus programs designed to engage young people in Rutgers University science and engineering programs. In addition, she helps university faculty to develop innovative and effective broader impact statements in accordance with NSF's Criterion II. Scientists and Engineers are engaged in a wide variety of education and outreach initiatives designed to educate the public about STEM disciplines. McDonnell works with scientists to translate their research into educational products that can be used by K-16 students, teachers and the general public. Finally, she is interested in program evaluation and works with a range of external collaborators to conduct a range of program assessments.



Kevin Hand

Kevin P. Hand is a planetary scientist and astrobiologist at NASA's Jet Propulsion Laboratory, where he directs the [Ocean Worlds Lab](#).

His research focuses on the origin, evolution and distribution of life in the solar system with an emphasis on moons of the outer solar system that likely harbor liquid water oceans. He is the pre-Project Scientist for NASA's Europa Lander mission concept and was co-chair of the 2016 Europa Lander Science Definition Team. From 2011-2016 Hand served as Deputy Chief Scientist for Solar System Exploration at JPL. His fieldwork has brought him to Antarctica, the Arctic, the depths of Earth's ocean, the glaciers of Kilimanjaro and Mt. Kenya, and the desert of Namibia. His book 'Alien Oceans: The Search for Life in the Depths of Space', was recently published by Princeton University Press.

Abstract: Alien Oceans: The Search for Life in the Depths of Space. A key discovery from the past six decades of solar system exploration is that liquid water oceans may be a common planetary phenomenon. At least six ice-covered moons of the outer solar system present compelling evidence for subsurface oceans, and as such provide highly compelling targets in our search for life beyond Earth, and for the nascent field of comparative oceanography. In this talk I will briefly describe several lines of evidence for these oceans, and then I will detail some of the latest discoveries made about Jupiter's moon Europa. I will also discuss how the exploration of these worlds can help inform our understanding of the origins of life. I will conclude with an overview of approved, and proposed, missions that will explore these worlds in the coming decades.