THE UNIVERSITY OF BRITISH COLUMBIA

2021 UBC Chemistry Graduate Research Symposium

Saturday, September 25th

10:00 AM– 4:30 PM

CHEMISTRY GRADUATE STUDENT SOCIETY

Plenary Lecture

Quantitative Modeling Tools for Prediction in Synthesis and Catalysis

When faced with an unfamiliar reaction space, synthetic chemists typically apply the reported conditions (reagents, catalyst, solvent, and additives) of a successful reaction to a desired, closely related reaction using a new substrate type. Unfortunately, this approach often fails owing to subtle differences in reaction requirements. Consequently, an important goal in synthetic chemistry is the ability to transfer chemical observations from one reaction to another. Therefore, we have aimed to develop a program that assists the rapid analysis of the general interactions that impart asymmetric induction allowing the quantitative transfer of this stereochemical information to new reaction components and mechanisms. This talk will outline how we have developed an approach that combines organic synthesis, quantum chemistry, and machine learning to predict and interpret reaction outcomes. Ultimately, these techniques enable models to be generated from one set of reactions that can be deployed to predict another, streamlining reaction and catalyst development.

Prof. Jolene P. Reid, UBC Department of Chemistry

Symposium Info

The Graduate Research Symposium is a great opportunity for UBC chemistry students and postdocs to share their latest research with their colleagues in the department. The 2021 UBC Chemistry Graduate Research Symposium will be held **in-person** within the UBC Chemistry Building.

Prizes will be awarded to the top three student poster presentations, as judged by faculty judges.

All event attendees must have proof of 1+ dose of an approved Covid-19 vaccine to attend the event. Masks are required for indoor portions of the event.

Schedule of Events

From 9:30	Continental Breakfast B-Wing Lobby
10:00 - 11:00	Plenary Lecture by Prof. Reid Room B250
11:00 - 11:30	CGSS General Meeting Room B250
11:30 - 1:00	Poster Session #1 Grad Lounge (D211), D-Wing Hallways
1:00 - 2:30	BBQ Lunch Break Courtyard Between B- and D-wing
2:30 - 4:00	Poster Session #2 Grad Lounge (D211), D-Wing Hallways
4:00 - 4:30	Closing Remarks & Prizes Room B250

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Poster Session #1

#	Presenter	Poster Presentation
1	*Abhishek Soni*	**Unravelling the Mechanism of Ice Nucleation by Mica (001) Surfaces** Heterogeneous ice nucleation is an important process in atmospheric science, food preservation, and other areas of research. Muscovite mica is a commonly occurring mineral and, although its ice nucleating ability has been widely debated, recent experiments have established that some mica (001) surfaces e ciently nucleate ice. We employ molecular dynamics simulations to investigate ice nucleation by three variations of the mica (001) surface. These are: bare surfaces devoid of counterions (B-mica); surfaces with ordered arrangements of K+ counterions (K-mica); and protonated surfaces (H-mica). Our simulations show that B-mica and H-mica effectively nucleate ice, but K-mica does not. For B-mica and H-mica, the ice nucleation mechanism is unusual in that it does not occur via the basal or prism plane of Ih. The mica (001) surfaces stabilize an ice bilayer resembling (but not identical to) the pyramidal (20-21) plane of Ih. This results in a mixed-phase ice nucleus consisting of hexagonal and cubic ice layers stacked in a particular order imposed by the surface. We discuss in detail the connections between surface composition, morphology, and ice nucleation. The in uence of nite system size on ice nucleation is also investigated. Finally, we discuss our simulations in view of recent experimental results. Taken together, the experiments and simulations cast new light on ice nucleation by mica (001) surfaces.
2	*Afagh Habibzadeh*	**A Reversible Redox Chemistry of In(III) to In(I)** Indium (I) species have been studied much less compared to their group 13 counterparts. Hence, here, synthesis and design of a series of NCN pincer complexes that stabilize and provide options for tuning and studying monomeric stable indium (I) complexes have been studied. DFT calculations for both indium (III) and indium (I) complexes proves that the planar and conjugated nature of the ligand can stabilize the complex and allow us to tune the Lewis acidity of indium (I) center without effecting the Lewis basicity of the system by tuning the functional groups of the ligand. Using the same ligand system, lead to discovery of a hemilabile indium complex.
3	*Alexandra McKinnon*	**UV Photolysis Study of Para-Aminobenzoic Acid Using pH_2 Matrix Isolation Spectroscopy** We present the photolysis of para-aminobenzoic acid (PABA) with three different UV ranges (UVA: 355 nm, UVB: > 280 nm, and UVC: 266 nm and 213 nm) isolated in solid parahydrogen (pH2) matrices. The nitrogen-centered PABA radical was the main primary photoproduct of PABA following > 280 nm, 266 nm, and 213 nm irradiation. Our results showed that PABA easily loses an amino hydrogen atom upon UVB and UVC light and that the PABA radical is relatively stable in our matrix for hours after irradiation. We identified the infrared spectrum of the PABA radical in solid pH2 for the first time and compared it with quantum chemical calculations. We also observed the trans-HOCO radical as a minor secondary photoproduct of PABA following 213 nm irradiation. We analyzed the photochemical products and their reaction dynamics using Fourier-Transform Infrared (FTIR) spectroscopy.

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Poster Session #1

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4	*Ali Shoja*	**Computational Insights into Privileged Stereocontrolling Interactions Involving Chiral Phosphates and Iminium Inter-** The reactivity landscape of chiral phosphate catalysis is rapidly expanding and currently ranges from the hydrogenation of enals to the electrophilic activation of allenamides. Despite the importance of such transformations for the stereocontrolled synthesis of a diverse array of organic compounds, the preferred pathway and reasons for stereocontrol have not been firmly established making it difficult to develop new reactions more generally. Here, we address this challenge by integrating traditional transition state calculations with statistical tools to rapidly connect and analyze several types of chiral phosphate catalyzed enantioselective transformations., Detailed DFT calculations of carefully selected case studies reveal that this set of superficially unrelated reactions operate, in many cases, through a single mechanism involving two hydrogen-bonding interactions from the iminium intermediate and nucleophile to the catalyst. From the transition state structures, we rationalize the different factors on which the enantioselectivity depends, focusing on the orientation of the reactants with respect to the catalyst. These theoretical analyses led to the construction of stereochemical models that correlate the magnitude and explain the sense of enantioselectivity for over 200 chemical reactions. We demonstrate how the resulting models can be used to assist reaction application to include additional substrates and develop related transformations. Ultimately, our findings represent a framework for formulating mechanistically relevant correlations driven by high-level transition state analysis and this strategy should be broadly applicable to other catalytic systems widely applied in asymmetric synthesis.
5	*Andrew Kukor*	**A Robust New Tool for Online Solution-Phase Sampling of Crystallizations** Current PAT tools struggle to provide real time solid-phase composition data for crystallizations since measurements are made in the solution phase. Combining total (solid plus solution phase) sampling with solution-only sampling can provide this data, but the selective solution-phase sampling of supersaturated solutions is extremely challenging. I have developed a dynamically flushed in situ filtration device that attaches to the tip of Mettler-Toledo's EasySampler probe and makes use of its mechanical motion to avoid surface fouling. Filter functionality was tested under both increasing and decreasing saturation, illustrating its accuracy, reliability and versatility. The utility of the filter tip was highlighted by monitoring the classical resolution of TBZ, an important drug precursor.
6	*Ben Nadeau*	**Hammett investigation of substituted aminoquinolines in nickel mediated C(sp3)-H activation of tertiary ureas** The 8-aminoquinoline directing group has received considerable attention for directed C-H bond activation of unactivated substrates. In recent reports, significant mechanistic insights into the nickel mediated C-H activation and cyclometallation have been uncovered via isolation of key intermediates along a proposed catalytic cycle. This work aims to expand on our previous mechanistic results by investigating the electronic factors of the aminoquinoline directing group, and its influence on nickel mediated C-H activation through a Hammett analysis. Initial experimental results produced a non-linear Hammett plot, and additional mechanistic insights indicate that the previously accepted mechanism of C-H activation may be more complex than previously proposed.
7	*Cameron Zheng*	**A tri-catalytic telescoped synthesis of indoles enabled by tantalum-catalyzed hydroaminoalkylation**

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Poster Session #1

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8	*Devin Klapatiuk*	**Extension of the Carbon-Carbon Sigma Bond Beyond 2 Angstroms**
9	*Diana Kim*	**Tuning the properties of lignin-graft-PLA nanofibers with tacticity**
10	*Hatsuki Otani*	**Search for superfluidity in large para-H2 clusters** Our group have been studying ultracold molecular parahydrogen (p-H2) clusters aiming to identify superfluid nature in the molecular clusters. By the use of mass and optical spectrometry, we identified fluxional nature of p-H2 clusters containing 10^5 molecules expanded in a vacuum chamber using a pulsed nozzle. Experimental details will be discussed in my poster.
11	*Hayden Scheiber*	**Machine Learns to Optimize LiX Forcefields** Nucleation is a microscopic event that initiates the transformation of one thermodynamic phase into another, ending with the most thermodynamically stable phase that's accessible. The process of crystallization begins with the nucleation of a microscopic crystal that grows outward rapidly. Molecular dynamics (MD) is a common computational chemistry technique employed for the study of nucleation, as nucleation often occurs on length- and time-scales too short to easily probe with experiments. In order to model realistic behaviour with MD, a suitable forcefield must be chosen that defines all interactions between the atoms in the system of interest. Although the best possible accuracy can be achieved by employing a full many-body quantum-mechanical forcefield, pairwise forcefields are ubiquitous in the literature as they greatly reduce the computational cost of MD, allowing for larger and longer chemical simulations. Simulations employing these simplified force fields are called classical MD simulations. One huge obstacle for the use of classical forcefields is the tuning of forcefield parameters to ensure a realistic simulation. Typically, researchers fit the parameters of forcefields to experimental or theoretical results. In this research, we generate useful pairwise model parameters for lithium halide salt nucleation research using Bayesian Optimization. By re-casting the problem of model parameter fitting into an optimization problem, and using targets produced from high accuracy quantum mechanical calculations, we are able to rapidly probe right to the limits of pairwise modeling in a complex chemical system.
12		(Presentation withdrawn)

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Poster Session #1

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13	*Jiacheng Zuo*	**Single Molecule Force Spectroscopy Studies of Missense Titin Mutations That Are Likely Causing Cardiomyopathy** The giant muscle protein titin plays important roles in heart function. Mutations in the titin have emerged as a major cause of familial cardiomyopathy. Missense mutations have been identified from cardiomyopathy patients; however, it is challenging to distinguish disease-causing mutations from those benign ones. Given the importance of titin mechanics in heart function, it is of critical importance to elucidate the mechano-phenotypes of cardiomyopathy-causing mutations found in the elastic I-band part of cardiac titin. Using single molecule AFM and equilibrium chemical denaturation, we investigated the mechanical and thermodynamic effects of two missense mutations R57C-I94 and S22P-I84 found in the elastic I-band part of cardiac titin that were predicted to be likely causing cardiomyopathy by bioinformatics analysis. Our AFM results showed that mutation R57C had a significant destabilization effect on I94 module. R57C reduced the mechanical unfolding force of I94, speed up the unfolding kinetics while slowed down folding kinetics. These effects collectively increased the unfolding propensity of I94, likely resulting in altered titin elasticity. In comparison, S22P only led to modest destabilization of I84, with a reduction of unfolding force by ~10 pN. It is unlikely that such a modest destabilization would lead to a change of titin elasticity. These results will serve as the first step towards elucidating mechano-phenotypes of cardiomyopathy-causing mutations in the elastic I-band.
14	*Jiayao Lu*	**Dithiocarbamate SAMs on Au and Cu: Tuning CO2 Reduction Activity through Molecular Functionalization**

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Poster Session #2

#	Presenter	Poster Presentation
15	*Jiayu Li*	**The Folding-Unfolding Mechanism of Cytochrome C Probed by Single-Molecule Optical Tweezers** Metalloproteins account for over one-third of all proteins in nature and play important roles in biological processes. The formation of the native structures of metalloproteins requires not only the correct folding of the polypeptide chains, but also the proper incorporations of metal cofactors, which makes the folding process even more complicated. Heme proteins are one of the most common metalloprotein families in nature and are highly versatile in their biological roles. Among them, cytochrome c (cytc), which contains a c-type heme cofactor, acts as an important electron transfer protein in both aerobic and anaerobic respiration processes. The folding mechanism of horse heart cytc has been extensively studied by ensemble spectroscopic methods. It was found that the holo-form (heme-bound) cytc (holo-cytc) folded into a helical structure, and the apo-form (heme-free) cytc (apo-cytc) showed no spectroscopic signals of folded structures. The heme cofactor was then believed to be decisive for the folding of cytc. Here, we used single-molecule optical tweezers to probe the mechanical folding-unfolding behaviors of holo-cytc and apo-cytc at the single-molecule level. Our results suggested that, holo-cytc demonstrates the typical folding-unfolding behaviors of a folded protein. Apo-cytc, which has been long believed to be random coiled, intriguingly displays some intrachain interactions and may fold into an ensemble of molten globule states. Therefore, the interactions between the heme cofactor and the polypeptide chain can facilitate the polypeptide chain folding and guide the protein to fold into the native state. Our results unambiguously demonstrated the mechanical folding-unfolding behaviors of holo- and apo-cytc, and bring new insights to our understanding of the folding mechanisms of heme proteins as well as the role of heme cofactors in the folding process.
16	*Kaeden Teindl*	**Relating the Acidity of Pendent Amides with CO2 Reduction Activity in a Series of Iron Porphyrin Electrocatalysts**
17	*Kimia Hosseini*	**Ligand Design for Catalysis by Cationic Indium Complexes** Ligands offer many opportunities for changing the stability and reactivity of catalysts. Previously, we reported that cationic indium complexes supported by ligands containing hemilabile moieties can be used to tune the stability and reactivity of indium complexes in synthesis of biodegradable polymers. In this project, we synthesize and characterize various cationic indium complexes and study their reactivities towards synthesis of spiro-ortho esters. Spiro-orthoesters are important monomers for making biodegradable polymers. We show that in these cationic complexes, alkyl groups with different bulkiness and polarizabilities have different reactivities in the synthesis of spiro-orthoesters. We aim to understand how modifications to the previously reported hemilabile moieties can affect the reactivity of indium complexes. These studies will help us explore the effect of ligand design on catalysis by cationic indium complexes.

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Poster Session #2

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18	*Mason Guy*	**Organic molecules as a downloadable digital object**
19	*Maxwell Thompson*	**Hydroaminoalkylation: A Synthetic Tool for Advancing Amino Acid Drug Discovery**
20	*McKenzie Madden*	**Synthesis of Nitrogen Rich Long Pendent Aminopolyolefins**
21	*Qingyuan Bian*	**Engineering Shape Morphing Protein Hydrogels Based on Protein Unfolding-Folding** Engineering shape morphing materials have achieved considerable progress in polymer-based systems, and have demonstrated potential applications in a broad range of fields. However, engineering protein-based shape memory/morphing materials remains challenging and under-explored. Here we report the engineering of protein-based shape memory/morphing hydrogels by utilizing protein folding-unfolding as a general mechanism to trigger shape-morphing in protein-bilayer structures. We used two different tandem modular elastomeric proteins (GB1)8 and (FL)8 as building blocks to engineer shape-memory/shape-morphing bilayer protein hydrogels. We found that the (GB1)8 and (FL)8 hydrogels displayed different Young's moduli and swelling properties. Upon chemical denaturation, these two hydrogels displayed denaturant-dependent swelling profiles that are different for these two hydrogels. Due to such unfolding-folding induced changes in swelling, the bilayer hydrogel displayed a bidirectional bending deformation depending upon the buffer condition. The bending orientation and angle showed strong dependence on the denaturant concentration and layer geometry, endowing the bilayer hydrogel tunable bending behaviors. Such shape morphing properties also exhibited excellent reversibility and stability. Based on its programmable and reversible bending behaviors, we further utilized the bilayer protein hydrogel as hinge to drive a folding deformation and realized one-dimensional (1D) to two-dimensional (2D) and 2D to three-dimensional (3D) transformations of patterned hydrogels. We believe the present work would offer new inspirations for the design and fabrication of novel shape morphing materials.
22	*Rida Farhat*	**Investigation of Metalloporphyrins for Electrochemical Reductive Desulfurization**
23	*Sasha Cryan*	**Exploring Electrochemical CO2 Reduction with Ruthenium Polypyridyl Complexes: Targeting Carbon-Carbon Bond Formation**
24	*Shanal Gunasekera*	**Rapid, High-Yielding Solid-Phase Synthesis of Cathepsin□B Cleavable Linkers for Targeted Cancer Therapeutics**

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25	*Siwei Luo*	**A lattice-mapped scheme with fuzzy switching functions** Coarse-grained (CG) models reduce the number of degrees of freedom in a system, allowing the dynamics of large systems to be studied for longer times. Many CG models have been developed since the way of generating a CG system highly depends on the question one is interested in. Standard CG models fail to study non-bonded particles since the motion of free particles disperses them and disintegrates the CG cluster. This issue can be solved by coarse-graining a system into lattice-like subcells where atomistic particles can dynamically change their contribution to any CG variable. In this work, CG potentials generated from a lattice-like mapping of non-bonded atomistic particles are studied. Fuzzy switching functions are used at the boundary of subcells to produce continuous CG trajectories. The behaviour of the potentials is examined while changing the fuzziness of the switching functions for Lennard-Jones(LJ) systems. In general, the CG potentials retain a quadratic form. Compared with the Heaviside switching function[1], correlations involving different vector components of CG positions, off-diagonal CG masses arise as a consequence of having a shared region between subcells. A few unique potential parameters are needed to construct the CG potentials for homogeneous LJ fluids. Understanding the CG potentials is a necessary part of developing a CG model for fluids. Such a model explores the connection between atomistic and continuum theories in which a general method may be found to simulate complex biological systems. [1] Luo, S.; Thachuk, M. Conservative Potentials for a Lattice-Mapped Coarse-Grained Scheme. J. Phys.
26	*Tianyu Duan*	**Light-Responsive Dynamic Protein Hydrogels Based on LOVTRAP** Protein-based hydrogels can mimic many aspects of native extracellular matrices (ECMs) and are promising biomedical materials that find various applications. To be adapted for different tasks, it is important that the mechanical or biochemical properties of protein-based hydrogels can be regulated by external stimuli. The non-covalent binding between the light-oxygen-voltage-sensing domain 2 (LOV2) and its binding partner ZDark1 (zdk1), named as LOVTRAP, is a light-responsive interaction. The affinity of LOVTRAP is much larger in dark than that under blue light irradiation. Taking advantage of this light-responsive interactions, we endeavored to use LOVTRAP as a crosslinking mechanism to engineer light responsive protein hydrogels. By using LOV2-containing and zdk1-containing multifunctional protein building blocks, we successfully engineered a light-responsive protein hydrogel whose viscoelastic properties can change in response to light: in the dark, the hydrogel showed higher storage modulus; under blue light irradiation, the storage modulus decreased. Due to the non-covalent nature of the LOVTRAP, the engineered LOVTRP protein hydrogels displayed shear-thinning and self-healing properties, and served as an excellent injectable protein hydrogel. We anticipated that this new class of light-responsive protein hydrogels will broaden the scope of dynamic protein hydrogels and help develop other light-responsive protein hydrogels for biomedical applications.

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Poster Session #2

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27	*Yi Ren*	**Effects of pH on Immersion Freezing by Kaolinite** Heterogeneous ice nucleation refers to ice nucleation initiated by an ice nucleating particle (INP). Important INPs include mineral dust particles and biological particles. Nucleation processes are affected by cloud conditions, for example, the cloud pH. Clouds are generally acidic and have a range of pH values. Alkaline particulates significantly increase the cloud water pH leading to near-neutral or even basic clouds. The effect of cloud pH on ice nucleation has not been extensively studied. We investigate the effect of pH on immersion freezing by kaolinite employing both droplet freezing experiments and molecular dynamics simulations. In droplet freezing experiments, kaolinite suspensions are mixed with various concentrations of HNO3/NaOH solutions to cover a wide pH range. Our laboratory experiments show that freezing temperatures are similar under acidic and neutral conditions but decrease under basic conditions. This suggests that kaolinite remains active under acidic conditions but partly loses its nucleating ability under basic conditions. To model kaolinite particles immersed under different pH conditions, modified kaolinite Al-surfaces are investigated using molecular dynamics simulations. The Al (001) surface undergoes protonation under acidic conditions and deprotonation under basic conditions. We simulate multiple surface proton coverages on the Al (001) surface, and relate the surface proton coverage to pH through pKa values reported in the literatures. The pH range for which we observe ice nucleation in simulations agrees well with our droplet freezing experiments.
28	*Ziwang Wei*	**Piperazic acid as the precursor to piperazate-containing non-ribosomal peptides**
29	*Edène Rocheron*	**Interferometric Scattering Microscopy System for the Characterization of Gold Nanoparticles**