14th ATLANTIC THEORETICAL CHEMISTRY SYMPOSIUM (ATCS 2017)

Hosted by the
Department of Chemistry, Dalhousie University
Halifax, Nova Scotia, Canada

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The Canadian Association of Theoretical Chemists

Chemical Institute of Canada | For Our Future
The Maritime Section of the Chemical Institute of Canada
The Physical, Theoretical and Computational Chemistry Division of the Chemical Institute of Canada
CONFERENCE LOCATION
Department of Chemistry, Dalhousie University
Chemistry Building, 6274 Coburg Rd, Halifax, NS B3H 4R2, Canada

TUESDAY AUGUST 1, 2017

2:20-2:40 PM
REGISTRATION/COFFEE Chemistry Room 225

2:40-4:00 PM:
TALKS Chemistry Room 226

SESSION CHAIR: Erin Johnson

2:40-3:20 PM
Richard Dawes*, Steve Ndengué, and Ernesto Quintas Sánchez: Calculations of Spectroscopy and Reaction Dynamics using interpolated ab initio Potentials

3:20-4:00 PM
Jayendran C. Rasaiah*: Ion transport in liquid water, nanotubes and water wires

4:00 PM-4:20 PM:
COFFEE BREAK Chemistry Room 225

4:20-5:30 PM:
TALKS Chemistry Room 226

SESSION CHAIR: Erin Johnson

4:20-5:00 PM
Tao Zeng*: Our recent studies on vibronic coupling: applications in singlet fission and paper-and-pen works on deriving Hamiltonians

5:00-5:30 PM:
Poster Flash Presentations (2 min per person)
TUESDAY AUGUST 1, 2017

6:30-8:30 PM
RECEPTION AND POSTER SESSION
Garrison Brewing Company
1149 Marginal Rd, Halifax, NS B3H 4P7, Canada

Directions to Garrison Brewing Company from Chemistry Building
From the Chemistry Building, head east on University Ave. (1.1 km).
Continue onto Morris St (0.7 km).
Turn right onto Hollis St (0.2 km).
Turn left onto Terminal Rd (0.4 km). Garrison Brewing Company will be on the left.

WEDNESDAY AUGUST 2, 2017

9:20-10:40 AM:
TALKS Chemistry Room 226
SESSION CHAIR: Gabriel Hanna

9:20-10:00 AM:
Jeremy Schofield*: Exploring the connection between thermodynamics, frustration and folding dynamics in simple chain models of a protein

10:00-10:20 AM:
Bryan Linford, Enrico Bodo, and Travis Fridgen*: Using molecular dynamics and density functional theory with infrared multiphoton dissociation to determine the structure of protonated beta-Methylamino-L-alanine

10:20-10:40 AM:
Csongor Matyas, and Raymond A. Poirier*: A new approach to characterize protein topology using knot projections

10:40 AM-11:00 PM:
COFFEE BREAK Chemistry Room 225

11:00 AM-12:40 PM:
TALKS Chemistry Room 226
SESSION CHAIR: Travis Fridgen

11:00-11:40 AM

11:40 AM-12:00 PM

12:00-12:20 PM
Evan T. Walters, and Christopher N. Rowley*: Evaluating dispersion interactions in molecular mechanical models for proteins and nucleic acids using the eXchange-hole dipole moment (XDM) model

12:20-12:40 PM
Matthew S. Christian, Alberto Otero-de-la-Roza, and Erin R. Johnson*: Adsorption of Graphene to Metal (111) Surfaces using the Exchange-Hole Dipole Moment Model

12:40-2:00 PM:
LUNCH
2:00-3:40 PM:
TALKS Chemistry Room 226

SESSION CHAIR: Aaron Kelly

2:00-2:40 PM
Holly Freedman, and Gabriel Hanna*: Modeling vibrational energy transport in molecules: Insights from mixed quantum-classical simulations of a model polypeptide

2:40-3:00 PM
Ernest Awoonor-Williams, and Christopher N. Rowley*: Computational Prediction of Cysteine pKa’s in Protein Kinases

3:00-3:20 PM
Yanyang Chen, Graham J. Bodwell, and Travis D. Fridgen*: Structures and energetics of metal cationized [1,1,n,n-tetramethyl[n](2,11)teropyrenophane] complexes (metal=Li, Na, K, Rb, Cs; n=8,9) studied by mass spectrometric and computational methods

3:20-3:40 PM
Zhe Li, D. Jean Burnell, and Russell J. Boyd*: Mechanistic Study on Cytochrome P450-Catalyzed C-H Amination

3:40-4:00 PM:
COFFEE BREAK Chemistry Room 225

4:00-5:20 PM:
TALKS Chemistry Room 226

SESSION CHAIR: Rustam Khaliullin

4:00-4:40 PM
Aaron Kelly*: Consumer Report on Simulation techniques for Charge and Energy Transfer in Chemistry: How to get the “most for your money” from Surface hopping, Mean Field Theory, and Master Equations

4:40-5:00 PM
Stephen G. Dale, Erin R. Johnson, and Axel D. Becke*: Interrogating the “B05” density functional for non-locality information

5:00-5:20 PM
Ernest Awoonor-Williams, Jennifer M. Smith, and Christopher Rowley*: Models for thiolates in the face of delocalization error and bad force fields

5:20-5:40 PM:
BUSINESS MEETING Chemistry Room 226

6:30 PM-TBD:
DINNER Dalhousie University Club
9:20-10:00 AM
Hayden Scheiber, Yifei Shi, and Rustam Z. Khaliullin*: Low-cost linear-scaling ab initio molecular dynamics

10:00-10:20 AM
Adam J. Proud, and Jason K. Pearson*: SEPDA - Single Electron Pair Distribution Analyser

10:20-10:40 AM
Ibrahim E. Awad, and Raymond A. Poirier*: Innovative way to build the molecular energies from atoms-in-molecules densities

10:40-11:00 AM
Mathew C. Larade, and Jason K. Pearson*: Applying Neural Networks to Predict Atomic Energies in Molecules

11:00-11:20 PM:
COFFEE BREAK Chemistry Room 225

11:20 AM-12:20 PM:
PANEL DISCUSSION Chemistry Room 226
Calculations of Spectroscopy and Reaction Dynamics using interpolated ab initio Potentials

Richard Dawes*, Steve Ndengué, and Ernesto Quintas Sánchez
Missouri University of Science and Technology, Rolla, Missouri, USA

Part of this talk describes the development of a PES generator (software code) which uses parallel processing on High-Performance Computing (HPC) clusters to construct PESs automatically. Thousands of ab initio data are computed at geometries chosen by the algorithm and fit to a functional form. The electronic structure of molecules is difficult to describe continuously across global reactive PESs since it changes qualitatively as bonds are formed and broken along reaction coordinates. I will discuss a high-level ab initio method (GDW-SA-CASSCF/MRCI) designed to allow the electronic wavefunction to smoothly evolve across the PES and provide an accurate and balanced description of the various regions.

These methods are combined with numerical methods to solve the Schrödinger equation for the nuclei in order to study a number of small gas-phased molecules from the areas of atmospheric, combustion and interstellar chemistry. Examples include DVR calculations of rovibrational levels as well as electronically nonadiabatic effects in photodissociation dynamics and inelastic scattering in HCO computed using the MCTDH method including the effects of Renner-Teller coupling.

References

Ion transport in liquid water, nanotubes and water wires

Jayendran C. Rasaiah*
Department of Chemistry, University of Maine, Orono, Maine, USA

We discuss the theory and simulations of ionic transport in water using non-dissociating (e.g. SPC/E) and dissociating water models (sOSS2); the latter based on a scaled interatomic potential (OSS2) derived by Ojamäe, Shavitt and Singer from ab-initio MP2 level calculations. The alkali metal and halide ions (Na⁺...Cs⁺, and F⁻...I⁻) show the distinct characteristic maxima as a function of radius displayed in experiments, attributed to hydrodynamic and dielectric friction. The dissociating model is just as easily applied to large systems as the classical non-dissociating models, and provides data in close agreement with quantum mechanical CP/MD and EVB calculations of proton transfer (PT). The H⁺ ion moves faster than the OH⁻ ions by nearly a factor of two, due to differences structural diffusion, and in excellent agreement with experiment from 0 to 50°C after correction to infinite dilution. The interaction energies the H⁺ or OH⁻ ion with a one-dimensional water-wire agrees closely with the dipole-lattice model of Dellago et al, and PT is much faster than in liquid water. Unlike bulk water, the diffusion of OH⁻ is slightly faster than H⁺ for short wires, but nearly the same for long wires, exhibiting the classic Grotthuss mechanism in the wire and not in liquid water. Recombination (neutralization) of H⁺ and OH⁻ in the open chain wire is accompanied by compression and a synchronized jump of three hydrogen-bonded protons at the final stages of neutralization, observed also by Hassanali et al in bulk water. Recombination in two-dimensions has yet to be fully explored.
Our recent studies on vibronic coupling: applications in singlet fission and paper-and-pen works on deriving Hamiltonians

Tao Zeng*
Department of Chemistry, Carleton University, Ottawa, Ontario, Canada

Singlet fission (SF) converts one short-lived singlet exciton to two long-lived triplet excitons, and can potentially enhance the photoelectric conversion efficiency in organic photovoltaic devices. In the new concept of intramolecular singlet fission (iSF), two chromophore units are covalently bonded and it is easier to adjust intermolecular morphology to facilitate SF. However, the detailed iSF mechanism is still unknown. In this presentation, two of our recent works in iSF are discussed.1,2 Through performing quantum chemistry calculations and quantum dynamics simulations, we investigated the general small size effects in iSF and presented a step-by-step picture for the through-linker iSF. With the new understanding, we propose a strategy to enhance the iSF efficiency by making appropriate substitution on the linker. In the second half of the talk, I will present our recent works on deriving general formalism of Jahn-Teller and pseudo-Jahn-Teller problems. More and more studies reveal that traditional second order expansions of the JT and pJT vibronic Hamiltonians in vibrational coordinates are inadequate. Our derivations for the general expansion formulas up to arbitrary order for trigonal3 and tetrahedral systems will be presented.

References
Exploring the connection between thermodynamics, frustration and folding dynamics in simple chain models of a protein

Jeremy Schofield

Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, Canada

A simple model of a protein-like chain is introduced to facilitate the exploration of the connection between the morphology of the free energy surface of the protein and its folding dynamics. A microscopic theory for the dynamics of the system is developed that reduces to a Markovian model of the kinetics under well-defined conditions. A helical-folding protein is constructed and its smooth free energy morphology is characterized. The dynamics of the system are analyzed within the Markov state model and it is demonstrated that the behavior of the equilibration profile as the temperature is lowered can be understood in terms of the initial formation of local structure through many pathways followed by more sequential passage through a series of configurations leading to the final structure. The effect of the presence of mis-folded states on the dynamics of the frustration is discussed.

Using molecular dynamics and density functional theory with infrared multiphoton dissociation to determine the structure of protonated beta-Methylamino-L-alanine

Bryan Linford\textsuperscript{a}, Enrico Bodo\textsuperscript{b}, and Travis Fridgen\textsuperscript{a,*}

\textsuperscript{a}Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

\textsuperscript{b}Department of Chemistry, Sapienza Universita Di Roma, Rome, Italy

Infrared multiphoton disassociation (IRMPD) spectroscopy is a useful method for determining the structures of gas phase ions, when coupled with computational methods. Common density functional theory (DFT) methods often provide a good spectral match for minimal computational effort, however there are cases where high anharmonicity can cause mismatches. In protonated beta-Methylamino-L-alanine (BMAA) a bridge is formed by one proton, causing significant N-H stretch broadening in the experimental spectrum which cannot be matched using DFT calculations. However, molecular dynamics (MD) simulations can be used to generate an infrared spectrum which accounts for this anharmonicity, resulting in a good match with the experimental work, and providing insight into the molecular structure.
A new approach to characterize protein topology using knot projections

Csongor Matyas, and Raymond A. Poirier*

Department of Chemistry, Memorial University, St. John’s, Newfoundland and Labrador, Canada

Protein folding is still a mystery, deeper understanding of protein topology is necessary. Although only some special cases of knotted proteins are known,¹,² these cases could help in the understanding of protein folding. Even if most proteins don’t fall in this special category, all protein look knotted at first and their projections can be characterized similarly. These knot projections can be used to measure similarity between the topology of any two protein. This can give some more insight on protein folding.¹,³

References


Atom-Centred Potentials: A Simple Approach Toward Improved Properties from Hartree-Fock and Density-Functional Theory Methods

Gino A. DiLabio¹,²,³,*

¹Department of Chemistry and Faculty of Management, University of British Columbia, Okanagan, Kelowna, British Columbia, Canada
²National Institute for Nanotechnology, National Research Council of Canada, Edmonton, Alberta, Canada

We have developed a new, low-cost approach to improve the accuracy of results obtained from Hartree-Fock and density-functional theory calculations. The approach makes use of atom-centred potentials (ACPs), which are similar in structure and used in the same way as effective core potentials. Instead replacing core electrons, our ACPs are designed to produce corrections to calculated energies that result in a remarkable improvement in a wide-range of calculated properties, either by mitigating the effects of basis set incompleteness error or the errors arising from incomplete correlation treatment, or both. The motivation for the use of ACPs for improved electronic structure calculations will be presented, along with examples demonstrating their performance for a variety of chemical systems.¹–³

References


Luc M. LeBlanc\textsuperscript{a}, Alberto Otero-de-la-Roza\textsuperscript{b}, and Erin R. Johnson\textsuperscript{a,∗}

\textsuperscript{a}Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada
\textsuperscript{b}Department of Chemistry, University of British Columbia, Okanagan, Kelowna, British Columbia, Canada

\textit{In silico} prediction of crystal structures (CSP) strictly from a molecular diagram is a challenging task. The difficulties, in part, lie in developing electronic structure methods that are accurate enough to capture small energy differences, while remaining computationally inexpensive. While the various low-cost approximate methods proposed in the literature\textsuperscript{1} provide a framework to tackle the issue, the levels of accuracy achieved for computed energy differences between structures are unsatisfactory; it can be argued that their accuracy is insufficient to rank polymorphs or candidate crystal structures in the context of CSP. We propose an alternative approach: using low-cost methods as a means of yielding geometries that are transferred to single-point energy calculations with higher-level methods. Provided the low-cost method gives reliable geometries, this removes the need to correct for any errors due to, e.g., localized basis sets. The same accuracies for lattice energies as if one had used the high-level method alone are then obtained. Applications to organic molecular solids and to preferential crystallization of chiral molecules will be presented.\textsuperscript{2}

References


Evaluating dispersion interactions in molecular mechanical models for proteins and nucleic acids using the eXchange-hole dipole moment (XDM) model

Evan T. Walters, and Christopher N. Rowley\textsuperscript{∗}

Department of Chemistry, Memorial University of Newfoundland, St. Johns, Newfoundland and Labrador, Canada

London dispersion interactions are a significant factor that define the structure and dynamics of proteins. By understanding and quantifying these interactions, a more complete understanding of the nature of protein folding can be attained and would help allow predictions of the folded structures of proteins. Molecular mechanical force fields such as CHARMM, AMBER, OPLS-AA, and the Drude polarizable force field assign fixed parameters to describe the dispersion interactions of the various atom types in proteins. These parameters can also be calculated using the exchange-hole dipole moment model (XDM). In many cases, the XDM-calculated atomic $C_6$ coefficients are vastly different from the force field parameters, and the dispersion parameters used by these force fields are widely varied. Nucleic acid structures are also influenced by dispersion interactions between nucleobases. Agreement between force field and calculated $C_6$ coefficients is also fairly poor for the nucleobases. This disagreement for both nucleobases and amino acid side chains highlights an unrecognized error in molecular mechanical descriptions of dispersion interactions in proteins and nucleic acids.
Adsorption of Graphene to Metal (111) Surfaces using the Exchange-Hole Dipole Moment Model

Matthew S. Christian\textsuperscript{a}, Alberto Otero-de-la-Roza\textsuperscript{b}, and Erin R. Johnson\textsuperscript{*a}

\textsuperscript{a}Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada
\textsuperscript{b}Department of Chemistry, University of British Columbia, Okanagan, Kelowna, British Columbia, Canada

Graphene is a material that has unique electronic and tribologic properties. Understanding how graphene interacts with metals is important for advancing the use of graphene beyond the laboratory test environment to commercial manufacturing. Until recently, modeling graphene’s interaction with metals using conventional density-functional theory (DFT) has been difficult because the lack of long-range, non-local correlation needed to calculate dispersion interactions. However, dispersion can be accounted for by adding a post-SCF correction to the DFT energy. We present a thorough study of graphene adsorption on metal surfaces using DFT, incorporating the exchange-hole dipole moment (XDM) dispersion model. Our results reproduce experimental observations of strong and weak graphene-metal interactions and demonstrate clear periodic trends. We also show that graphene typically prefers an aligned orientation with the metal surface and highlight how carbon-carbon bond strain affects monolayer formation.

References


Modeling vibrational energy transport in molecules: Insights from mixed quantum-classical simulations of a model polypeptide

Holly Freedman\textsuperscript{a}, and Gabriel Hanna\textsuperscript{b,*}

\textsuperscript{a}Department of Medical Microbiology and Immunology, University of Alberta, Edmonton, Alberta, Canada
\textsuperscript{b}Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada

Intramolecular and intermolecular vibrational energy transport (VET) processes are ubiquitous in chemistry and biology. In some cases, a detailed understanding of the speed, mechanism, and efficiency of the VET may be obtained through classical molecular dynamics simulations. However, how does one treat systems when the transport is quantum in nature? In this presentation, I will assess the validity of several mixed quantum-classical dynamics techniques for simulating VET, within the context of a 1D model of a polypeptide. In particular, I will compare the population dynamics of the amide I modes (induced by an infrared excitation of the first mode in the polypeptide), simulated via the Ehrenfest method and three solutions of the quantum-classical Liouville equation (QCLE)–namely, a surface-hopping solution, an adiabatic solution, and the Poisson Bracket Mapping Equation (PBME) solution.\textsuperscript{1} When the frequencies of the amide I modes are equal, surface-hopping and adiabatic dynamics give rise to an even redistribution of the excitation energy from the first amide I mode onto the remaining modes on a timescale of a few hundred femtoseconds, while PBME and Ehrenfest dynamics predict energy delocalization on a picosecond timescale. In contrast, when the frequencies of the amide I modes at each end of the polypeptide are equally increased with respect to those of the remaining modes, surface-hopping and adiabatic dynamics give rise to a direct hopping of the energy from one end of the polypeptide to the other, while no transport is observed in the PBME and Ehrenfest cases. In light of the more accurate nature of the surface-hopping solution, these results demonstrate that the PBME and Ehrenfest approaches fail for modeling this VET process. These findings hold promise for simulations of VET in more realistic systems via the surface-hopping and adiabatic solutions of the QCLE.

References

Computational Prediction of Cysteine pKₐ’s in Protein Kinases

Ernest Awoonor-Williams, and Christopher N. Rowley

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

The protein kinase family of signalling enzymes has over the years become a prolific target of inhibition for therapeutics, particularly cancer treatments.¹ Traditionally, most drugs bind to their targets through non-covalent interactions like hydrogen bonding. Recently, there has been renewed interest among drug developers and medicinal chemists to design drugs that bind covalently to their targets,² since these drugs tend to be more therapeutically potent than conventional non-covalent binding drugs. However, the vast number and structural similarity of protein kinases in the human kinome makes it difficult to design covalent-binding drugs that can selectively target particular kinases. Covalent-binding kinase inhibitors typically target cysteine residues within the active site of proteins. In principle, cysteines with low pKₐ values will be more susceptible to covalent modification since the nucleophilic thiolate is more accessible for binding. Identifying which cysteines in a given kinase that are readily accessible for covalent modification is a major challenge for drug developers, and most computational methods lack the desired accuracy in predicting cysteine reactivity in proteins.³ I will present an overview of current efforts that we are undertaking to predict the reactivity of druggable cysteines in the active sites of protein kinases.

References


Structures and energetics of metal cationized [1,1,n,n-tetramethyl[n](2,11)teropyrenophane] complexes (metal=Li, Na, K, Rb, Cs; n=8,9) studied by mass spectrometric and computational methods

Yanyang Chen, Graham J. Bodwell, and Travis D. Fridgen

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

1,1,n,n-tetramethyl[n](2,11)teropyrenophane (TMnTP) where n=8,9 present sizable cavities that molecules or ions can occupy. In this study, host-guest complexes composed of the TMnTP and metal cations are studied by both experimental and computational methods. Acetonitrile solutions of the metal cation and TMnTP are volatilized by electrospray ionization and are trapped and analyzed in a Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer which can be thought of as a test tube for gaseous ions. Their gas-phase structures are explored by sustained off-resonance irradiation collision-induced dissociation (SORI-CID) spectroscopy, blackbody infrared radiative dissociation (BIRD) kinetics, and infrared multiphoton dissociation (IRMPD) spectroscopy. B3LYP/6-31+G(d,p) calculations used to perform geometry optimizations and frequency calculations in Gaussian 09. One of the main purposes of these studies is to discern whether the ions might be inside or outside the TMnTP in the ion-molecule complex.
Mechanistic Study on Cytochrome P450-Catalyzed C-H Amination

Zhe Li, D. Jean Burnell, and Russell J. Boyd*

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

Cytochrome P450 enzymes can efficiently catalyze many C-H functionalizations. In the current study, the mechanism of P450-catalyzed C-H amination of aryl sulfonyl azides is being computationally probed. Amber-type force field parameters were developed for the heme and the substrate to enable the molecular dynamics simulation of the enzyme. The QM/MM (ONIOM) method was used to locate the transition states of the reactions and to calculate their activation barriers. The active species of the enzyme is the imidoiron(IV) compound (1) with a triplet electronic state. The C-H activation undergoes a stepwise pathway, which includes the hydrogen atom abstraction to produce the diradical (2), and then the diradical rebinds to generate the product (3). The radical re-binding step was calculated to be the rate-determining step. The calculated barriers are consistent with observed regio- and stereo-selectivity. The regio-selectivity was explained by the stabilization effect from the hydrogen bond between GLY 262 and the sulfone oxygen of the substrate.

References


Consumer Report on Simulation techniques for Charge and Energy Transfer in Chemistry:
How to get the “most for your money” from Surface hopping, Mean Field Theory, and Master Equations

Aaron Kelly

*Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

bTheory Department, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Approximate quantum dynamics methods offer a hierarchy of approaches to treat nonadiabatic processes like charge and energy transfer in chemical systems. Each tier of this hierarchy typically offers a different balance between accuracy and computational cost. However, for nonadiabatic problems containing large quantum subsystems, or where an on-the-fly treatment of the electronic states is required, only the lowest tiers of this hierarchy are likely to be practical, both now and in the foreseeable future. In this talk I will discuss how various approximate dynamics methods can achieve high levels of accuracy while retaining a very low computational cost, when they are utilized within a master equation approach. I will also demonstrate the massive advantages of this hybrid approach for applications ranging from an electron transfer reaction in solution, to electronic energy transfer in model photosynthetic systems.
Interrogating the “B05” density functional for non-locality information.

Stephen G. Dale, Erin R. Johnson, and Axel D. Becke

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

In two papers, Becke introduced Kohn-Sham density-functional approximations for static and dynamic correlation to be partnered with 100 percent exactly-computed exchange. Known as “B05”, this was the first non-local correlation model designed to work with the full non-locality of exact (or Hartree-Fock) exchange. Non-locality issues, often referred to as the “delocalization” problem, have emerged as one of the most vexing problems in DFT today. Questions such as... how much exact exchange should be used in a hybrid functional, or... what value of the range parameter should be used in a long-range corrected functional, abound, and the answers are system dependent. The physics of non-locality is built into the B05 functional in a natural way and one wonders, therefore, if B05 might provide a mechanism to answer such questions. Preliminary work exploring a procedure, “B05min”, to do this.

References

Models for thiolates in the face of delocalization error and bad force fields

Ernest Awoonor-Williams, Jennifer M. Smith, and Christopher Rowley

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

Thiols are present in biological systems, most notably as the side chain of cysteine amino acids in proteins. Thiols can be deprotonated to form a thiolate, which allows affords a diverse range of enzymatic activity and chemical modification of proteins. Modeling chemical reactions involving thiolates is surprisingly complex, as conventional DFT functionals like B3LYP and PBE are unable to reasonable mechanisms for some thiolate reactions. This is due, in part, to delocalization error, which is severe for weakly bound anions like thiolates. We found that range separated DFT functionals such as wb97x-D largely resolved these issues. We developed an automated workflow to model the addition of thiols to electrophiles and found a limited range of pharmaceutically-compatible electrophiles. QM/MM MD simulations of methylthiolate show that the thiolate anion is more diffuse than a sulfur, which is not well-described by some popular protein force fields.

References
Low-cost linear-scaling *ab initio* molecular dynamics

Hayden Scheiber, Yifei Shi, and Rustam Z. Khaliullin*
Department of Chemistry, McGill University, Montreal, Quebec, Canada

Despite remarkable recent progress in linear scaling density function theory, the computational cost of existing methods remains too high for routine *ab initio* molecular dynamics (AIMD) simulations. We developed a linear-scaling AIMD method with low computational overhead by utilizing compact molecular orbitals strictly localized within predefined radii. High efficiency of the method is achieved without sacrificing its accuracy with a combination of two techniques: (1) on-the-fly construction of accurate localized orbitals without lengthy self-consistent optimization and (2) the unbalanced Langevin integrator that is fine-tuned to retain stable dynamics even with imperfect forces. A remarkable feature of the implemented method is that it remains efficient even for challenging condensed phase systems even if large diffuse basis sets are used. We demonstrated that, for systems well-represented by the compact orbitals (e.g. molecular systems, ionic salts), the new AIMD method enables simulations on previously inaccessible time and length scales. The first steps towards generalizing the method to more challenging systems of strongly interacting atoms (e.g. covalent crystals) will also be discussed.

SEPDA - Single Electron Pair Distribution Analyser

Adam J. Proud, and Jason K. Pearson*
Department of Chemistry, University of Prince Edward Island, Charlottetown, Prince Edward Island, Canada

Electron pairs are at the heart of chemistry; however, understanding them is far from trivial. It is the two-electron component to the Schrödinger equation that makes it effectively impossible to solve. While our research doesn’t propose a way to solve this complex problem, it does provide insight into how electron pairs behave within molecules. Unlike much past research, we are not concerned with electron behaviour in the molecule as a whole, but in localized regions familiar to all chemists: bond and lone pair molecular orbitals. In this talk, I will discuss the software package SEPDA,\(^1\) which has the capability of calculating a variety of electron pair distribution functions\(^2\text{-}^3\) to analyze electronic distributions within covalent bonds and lone pairs. To date, SEPDA has been used to explore properties of first and second row hydrides, dative bonds, benzoic acid derivatives, hydrogen bonding interactions, 3c-2e\(^-\) bonds, and to monitor changes throughout the course of chemical reactions. This talk will highlight the capabilities of SEPDA, the areas where it has been applied, and the plans for the future of this software package.

References

Innovative way to build the molecular energies from atoms-in-molecules densities

Ibrahim E. Awad, and Raymond A. Poirier*

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

Computing the properties of large molecules by computing the properties of its atoms (atomic basins) or by generating them from small building blocks is a challenging problem in quantum chemistry. For example, properties of proteins could be computed by calculating the properties of their amino acids. The electron densities and some properties for atoms in molecules will be stored as a database. The electron density of a molecule of interest will be built using this database. As a result, the molecular properties (such as number of electrons, potential energy, etc) could be computed.

References


Applying Neural Networks to Predict Atomic Energies in Molecules

M. C. Larade, and Jason K. Pearson*

Department of Chemistry, University of Prince Edward Island, Charlottetown, Prince Edward Island, Canada

We present a novel method of predicting molecular energies using a summation of atomic energies, accurately predicted by feed-forward neural networks. This work attempts to combat the prohibitive scaling with respect to molecular size that restricts modern ab initio and density functional methods. To afford predictions of total molecular electronic energies of molecules of arbitrary size, we focus on predicting a priori the accurate energies of individual atoms, rather than whole molecules. To justify this approach, we employ the Quantum Theory of Atoms in Molecules (QTAIM). QTAIM states that the total electronic energy of a molecular system can be derived by summing all of the individual atomic energies within the system. In practice, however, it is difficult to accurately calculate the energy contribution of an individual atom without first calculating the energy of the molecule that contains it. In our approach, we have generated atomic energy data from 6000 small organic molecules consisting of carbon, oxygen and hydrogen to train a deep neural network for predicting atomic energies from the atomic environment. These machine-learned models should then be able to predict the energy contributions of individual atoms with the intent to sum them and attain accurate energy predictions for molecules of arbitrary size. Preliminary results show percent errors of 0.06%, 0.13% and 0.18% for carbon, hydrogen and oxygen atoms respectively.
A computational mechanistic study of the deamination reaction of melamine

Abd Al-Aziz A. Abu-Saleh, Raymond A. Poirier, and Mansour H. Almatarneh

aDepartment of Chemistry, Memorial University, St. John’s, Newfoundland and Labrador, Canada
bDepartment of Chemistry, University of Jordan, Amman 11942, Jordan

A detailed computational study of the deamination reaction of melamine by OH\(^{-}\), nH\(_2\)O/OH\(^{-}\), nH\(_2\)O (where n = 1, 2, 3), and protonated melamine with H\(_2\)O, has been performed using density functional theory and ab initio calculations. All structures were optimized at M06/6-31G(d) level of theory, as well as with the B3LYP functional with each of the basis sets: 6-31G(d), 6-311G(d), 6-31G(2df,p), and 6-311++G(3df,3pd). B3LYP, M06, and xB97XD calculations with 6-31+G(d,p) have also been performed. All structures were optimized at B3LYP/6-311G(d,p) level of theory for deamination simulations in an aqueous medium, using both the polarizable continuum solvation model and the solvation model based on solute electron density. Single point energy calculations have been conducted at G4MP2 and CBS-QB3. Fifteen different mechanistic pathways were explored. Most pathways consisted of two key steps: formation of a tetrahedral intermediate and in the final step, an intermediate that dissociates to products via a 1,3-proton shift. The lowest overall activation energy, 111 kJ mol\(^{-1}\) at G4MP2, was obtained for the deamination of melamine with 3H\(_2\)O/OH\(^{-}\).

References

Simple Model to Predict Correlation Energy of Closed- and Open-Shell Molecules

Ahmad. I Alrawashdeh, and Raymond A. Poirier

aDepartment of Chemistry, Memorial University, St. John’s, Newfoundland and Labrador, Canada
bDepartment of Physics and Physical Oceanography, Memorial University, St. John’s, Newfoundland and Labrador, Canada

The electron correlation energy has a significant importance in both wavefunction and density functional electronic structure theories. The methods that accurately account for the correlation energy are impractical and computationally expensive. Simple and practical model that is computationally efficient in computing the correlation energy for both closed- and open-shell molecules has been investigated. In this model, the electron correlation energy for molecules is described as a function of differences between atoms in molecule densities calculated at the nuclei and isolated atomic densities. The HF method with relatively a small basis set is the only method used in developing this model. The performance of this model was evaluated by comparing its predicting correlation energies for 56 small molecules with the exact correlation energies 1 using the root mean square deviation (RMSD) and \(R^2\). The model gives RMSDs of 9.6 \(\times\) 10\(^{-6}\) and 7.4 \(\times\) 10\(^{-5}\) for closed-shell and open-shell molecules, respectively.

References
Optimizing molecular properties by in-silico molecular evolution

René Fournier*, and Harneet Dhillon
Department of Physics and Astronomy, York University, Toronto, Canada

We used a global optimization (GO) strategy that optimizes molecular property with respect to both geometry and chemical composition. Our method combines features of genetic algorithm, taboo search, and memetic algorithm. A Relative Index of Thermodynamic stability (RITS)\(^1\) is used to make meaningful energy comparisons between different species. We did global optimization to minimize an objective function \(F_{ob} = RITS - cE_g\), where \(E_g\) is the HOMO-LUMO gap and \(c\) is a positive constant. The calculations were done for 130 bimetallic \(A_mB_n(5 \leq m + n \leq 8, A, B = Li, Mg, Al)\) and ternary species \(A_pB_qC_r(5 \leq p + q + r \leq 8, A, B, C = Li, Mg, Al)\). This was followed by local optimizations. All energy calculations were done with the Gaussian09 software at the PBE level of theory with LANL2DZ basis sets. Mg\(_4\)Al\(_4\), LiMg\(_2\)Al\(_5\), Li\(_2\)Al\(_6\), Li\(_2\)MgAl\(_5\), Mg\(_8\) with 20, 20, 20, 19 and 16 electrons respectively were ranked as the most stable species among the set. Frequency calculations verified these clusters as minima of potential energy surface. The highest HOMO-LUMO gap was found to be 1.76 eV for Mg\(_2\)Al\(_6\). The HL gaps for the most stable species Mg\(_4\)Al\(_4\), LiMg\(_2\)Al\(_5\), Li\(_2\)Al\(_6\), Li\(_2\)MgAl\(_5\), Mg\(_8\) are 1.355, 1.589, 1.678, 0.343 and 0.816 eV respectively.

References


Four Component Relativistic Wavefunction Program for Graphics Cards

Dylan Hennessey, and Mariusz Klobukowski*
Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada

General purpose computing with graphics cards is rapidly gaining in popularity and has seen widespread application and success in the high performance computing community. For computational chemistry, programs such as GAMESS and TeraChem have designed very efficient algorithms to attack the computational bottleneck that is two-electron integral evaluation as well as matrix diagonalization.\(^{1,2}\) This talk covers the process of porting over existing Fortran code into CUDA Fortran. We demonstrate its effectiveness by showing that we have achieved a 18x speed up of two-electron integral evaluation in the DFRATOM 4-component relativistic wavefunction program with calculations carried out in full double precision, fully reproducing results of calculations done on a CPU.\(^3\)

References

The Effect of Charge-Transfer Excitations on London Dispersion
Frederick W. G. Hills and Erin R. Johnson
Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

Photon-induced charge-transfer (CT) excitation is featured in a wide range of naturally occurring and synthetic dyes, many of which are of great utility in fields such as energy conversion and biomedical engineering. Time-dependent density-functional theory (TD-DFT) is the major theoretical tool currently used in studies involving excited states. In this work, TD-DFT is used to investigate the CT excitation in a series of known push-pull dye systems. Efforts are made to probe the effects of CT excitation on molecular properties related to London dispersion in the aforementioned systems. In particular, the changes in molecular $C_6$ dispersion coefficients are evaluated using the exchange-hole dipole moment (XDM) dispersion model. We speculate that, in the condensed phase, changes in dispersion interactions with neighboring molecules could significantly shift the energy of the CT excitation.

Improving the Genetic Algorithm on the Atomic Simulation Environment (ASE) Through Intelligent Starting Population Creation
Nicholas Kellas, and Michael N. Groves
Department of Chemistry and Biochemistry, California State University Fullerton, Fullerton, California, USA

The ASE genetic algorithm provides a means to find the lowest energy conformation of a molecule of a given stoichiometry. Our goal is to improve how the genetic algorithm creates its starting population, which should lead to faster, more efficient convergence to the global minimum. Our strategy is to have a population creator to form molecules based on the possible hybridized orbitals of each atom before using a clustering program to group similar structures together. Drawing structures from each group provides a much higher variety of possible configurations to the starting population. C9H7N was used as the molecular stoichiometry because the global minimum is known (quinoline), the potential energy surface is well explored, and finding the global minimum is not trivial from a random starting population due to quinoline’s ring structure. We will discuss details surrounding how our intelligent starting population generator alters the performance of the genetic algorithm as compared to when the starting population is created randomly and how consistently it is able to sample all available structures of molecules that the given stoichiometry can form.

References
Structures of $\beta$-methylamino-L-alanine isomers in the gas phase by IRMPD spectroscopy in the O-H/N-H stretching region and comparison of computational methods

Kelsey J. Menard, Bryan D. Linford, and Travis D. Fridgen*

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

The structures of protonated isomers of $\beta$-methylamino-L-alanine (BMAA) were investigated in the gas phase using Infrared multiple photon dissociation (IRMPD) spectroscopy in the O-H/N-H stretching region (2700-3800 cm$^{-1}$) in a Fourier transform ion cyclotron resonance mass spectrometer. Density functional theory (DFT) calculations for protonated 2,4-diaminobutanoic acid (2,4-DAB), protonated N-(2-aminoethyl)glycine (AEG), and protonated 3,4-diaminobutanoic acid (3,4-DAB) were performed using M06-2X and B3LYP methods with a 6-31G+(d,p) basis set. The computed IR spectra of the lowest energy protonated isomers of BMAA were then compared with experimental data. In addition, computational calculations of another BMAA isomer, protonated $\beta$-amino-N-methyl-alanine (BAMA), were performed using the M06-2X and the B3LYP methods. Comparison of the M06-2X and B3LYP methods revealed similar spectra when B3LYP spectra were scaled by 0.95 and the M06-2X spectra were scaled by 0.933 to compare with the IRMPD spectra in the N-H/O-H stretching region for the protonated isomers: 2,4-DAB, AEG, and 3,4-DAB

Calculation of Force Field London Dispersion Coefficients Using the Exchange-Dipole Model

Mohamad Mohebifar*a, Erin R. Johnsonb, and Christopher N. Rowley*a,*

aDepartment of Chemistry, Memorial University of Newfoundland, St. Johns, Newfoundland and Labrador, Canada

bDepartment of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

London dispersion interactions are of great importance in understanding phenomena such liquid properties, protein folding, and lipid structure. Force fields for molecular simulations of these systems typically determine the parameters for these interactions empirically. These parameters are generally underdetermined and there is no straightforward way of determining if they are physically realistic. The exchange-dipole model (XDM) from density functional theory can predict atomic London dispersion coefficients from first principles. We used this model to obtain the London dispersion coefficients of over 300 organic molecules relevant to biochemistry and pharmaceutical chemistry. We compared the XDM-calculated dispersion coefficients with the coefficients derived from the dispersion component of the Lennard-Jones parameters of the OPLS, CHARMM, AMBER, and Drude force fields. Generally, the force fields overestimate the $C_{6}$ dispersion coefficient. Also, there is a large range of dispersion coefficients for some atom types, which the force field models assume to be identical. XDM is a promising method to parameterize the dispersion terms of molecular mechanical force fields.

References

Development of atom-centered potentials approach for faster, efficient and accurate modeling of large molecular systems

Viki Kumar Prasad\textsuperscript{a}, Alberto Otero-de-la-Roza\textsuperscript{a}, and Gino A. DiLabio\textsuperscript{a,b,c,*}

\textsuperscript{a}Department of Chemistry, University of British Columbia, Okanagan, Kelowna, British Columbia, Canada
\textsuperscript{b}Faculty of Management, University of British Columbia, Okanagan, Kelowna, British Columbia, Canada
\textsuperscript{c}National Institute for Nanotechnology, National Research Council of Canada, Edmonton, Alberta, Canada

Accurate modeling of large molecular systems like supramolecular host-guest complexes, macromolecules, and water clusters are still a challenge for existing computational methods. The computational study of large systems requires a correct quantum mechanical treatment of both covalent and non-covalent interactions. However, this usually requires a computationally expensive approach such as a high-level correlated wavefunction method along with very large basis sets. Here, we propose a low-cost computational methodology based on dispersion-corrected Hartree-Fock (HF-D3) combined with a minimal basis set (MINIs). In order to correct for missing correlation interactions and for basis-set incompleteness error, we employ newly developed atom-centered potentials (ACPs), specifically fitted to reproduce high-quality wavefunction results. The combined approach adds little overhead to the computational cost and allows for the calculation of systems with up to thousands of atoms. The ACP approach is accurate and applicable with any electronic structure software package capable of using effective core potentials. In this work, we demonstrate how ACPs can be used for accurate modeling of noncovalent interactions, conformational changes and geometries of large molecular systems, with particular emphasis on water clusters.

Dispersion-Corrected DFT Study of Enantiospecific Adsorption of Amino Acids on Hydroxylated Quartz Surfaces

Alastair Price, and Erin R. Johnson\textsuperscript{*}

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

The chirality of amino acids is an important issue facing modern science with a further need to understand how controlled growth of enantiopure crystals can be achieved experimentally.\textsuperscript{1} Hydroxylated quartz surfaces have been shown to preferentially bind specific enantiomers of amino acids, making it suitable for enantiospecific separations.\textsuperscript{2,3} We extend the current understanding of the interaction of amino acids with these surfaces by using dispersion-corrected DFT methods, e.g., B86bPBE-XDM.\textsuperscript{4} In addition, we contrast the use of planewave approaches and low cost methods to perform these calculations. This work can be used as a stepping stone to provide further insight into how the amino acid crystal interacts with this surface.

References

The Charmm Lipid Force Field Can Be Used With More Accurate Water Models

Fatemeh Sajadi, and Christopher N. Rowley*

Department of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada

The CHARMM36 force field for lipids is widely used in simulations of lipid bilayers. The CHARMM family of force fields were developed for use with the TIP3P water model. This water model has an anomalously high dielectric constant and self-diffusion coefficient, which limits its accuracy in the calculation of quantities like permeability coefficients. The TIP3P-FB and TIP4P-FB are reparameterized water models that are more accurate in terms of the dielectric constant and transport properties, which could allow more accurate simulations of systems containing water and lipids. To test whether the CHARMM36 lipid force field is compatible with the TIP3P-FB and TIP4P-FB water models, we have performed simulations of DPPC and POPC bilayers. The calculated headgroup area, order parameters, and density profiles are in good agreement with the experimental values, suggesting that these improved water models can be used with the CHARMM lipid force field without modification.

Conformational analysis of ATP and its role in the phosphorylation mechanism of glucose

Andrew G. Walsh, Arpita Yadav, and Raymond A. Poirier*

aDepartment of Chemistry, Memorial University of Newfoundland, St. John’s, Newfoundland and Labrador, Canada
bDepartment of Chemistry, University Institute of Engineering and Technology Chhatrapati Shahaji Maharaj University, Kanpur 208024, India

There has been extensive research looking for new methods to combat organisms having different resistance mechanisms. One approach involves preventing adenosine triphosphate (ATP) phosphorylation by designing drugs having little binding ability with ATP, such as different conjugates of kanamycin, which keeps the drugs intact. In this study, we examine the energies and structures of the various ATP conformers, as well as a newly discovered isomer, both in the gas phase and in water using both DFT and HF methods with and without diffuse functions for comparison. The newly discovered isomer having a proton transferred from the ribose sugar to one of the oxygens of the beta phosphate group was consistently lower in energy than the other conformers both in the gas phase and in water. The phosphorylation reaction of each of the various conformers with glucose will also be discussed.

References


DFT-XDM modelling of electrolytes on graphite surfaces

Elias Zoghaib, and Erin R. Johnson*

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada

Ionic liquids are defined as organic salts with a boiling point below 100°C and play an important role as solvents in battery electrolytes for Li-ion and Li-air batteries. Despite numerous studies on these ionic liquids and their interactions on solid electrodes, little is known about the formation of the solid electrolyte interface (SEI) formed at the electrodes during the first few cycles of a battery. The SEI plays an important role for battery performance on the molecular scale. Density functional theory (DFT) can be used to model the SEI as well as describe the role of dispersion of the intermolecular interactions at the surface of the electrode. The exchange-hole dipole moment (XDM) method uses the interaction of induced dipoles to model dispersion. This talk outlines the use of XDM to model the interactions of several common electrolytes on the graphite anode of a battery to determine the adsorption energy in forming the SEI.
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<th>NAME</th>
<th>AFFILIATION</th>
<th>E-MAIL ADDRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abd Al-Aziz Abu-Saleh</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:aabusaleh@mun.ca">aabusaleh@mun.ca</a></td>
</tr>
<tr>
<td>Ahmad Alrawashdeh</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:aia638@mun.ca">aia638@mun.ca</a></td>
</tr>
<tr>
<td>Ibrahim Awad</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:iawad@mun.ca">iawad@mun.ca</a></td>
</tr>
<tr>
<td>Ernest Awoonor-Williams</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:esaw83@mun.ca">esaw83@mun.ca</a></td>
</tr>
<tr>
<td>Axel Becke</td>
<td>Dalhousie University</td>
<td><a href="mailto:axel.becke@dal.ca">axel.becke@dal.ca</a></td>
</tr>
<tr>
<td>Matthew Christian</td>
<td>Dalhousie University</td>
<td><a href="mailto:mchristian@dal.ca">mchristian@dal.ca</a></td>
</tr>
<tr>
<td>Stephen Dale</td>
<td>Dalhousie University</td>
<td><a href="mailto:stephen.dale@dal.ca">stephen.dale@dal.ca</a></td>
</tr>
<tr>
<td>Richard Dawes</td>
<td>Missouri University of Science and Technology</td>
<td><a href="mailto:dawesr@mst.edu">dawesr@mst.edu</a></td>
</tr>
<tr>
<td>Harneet Dhillon</td>
<td>York University, Toronto</td>
<td><a href="mailto:harneet2@yorku.ca">harneet2@yorku.ca</a></td>
</tr>
<tr>
<td>Gino DiLabio</td>
<td>University of British Columbia, Okanagan</td>
<td><a href="mailto:gino.dilabio@ubc.ca">gino.dilabio@ubc.ca</a></td>
</tr>
<tr>
<td>Travis Fridgen</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:tfridgen@mun.ca">tfridgen@mun.ca</a></td>
</tr>
<tr>
<td>Gabriel Hanna</td>
<td>University of Alberta</td>
<td><a href="mailto:gabriel.hanna@ualberta.ca">gabriel.hanna@ualberta.ca</a></td>
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<tr>
<td>Dylan Hennessey</td>
<td>University of Alberta</td>
<td><a href="mailto:dhennesse@ualberta.ca">dhennesse@ualberta.ca</a></td>
</tr>
<tr>
<td>Erin Johnson</td>
<td>Dalhousie University</td>
<td><a href="mailto:erin.johnson@dal.ca">erin.johnson@dal.ca</a></td>
</tr>
<tr>
<td>Nicholas Kellas</td>
<td>California State University, Fullerton</td>
<td><a href="mailto:nickellas094@csu.fullerton.edu">nickellas094@csu.fullerton.edu</a></td>
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<tr>
<td>Aaron Kelly</td>
<td>Dalhousie University</td>
<td><a href="mailto:aaron.kelly@dal.ca">aaron.kelly@dal.ca</a></td>
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<tr>
<td>Rustam Khalilullin</td>
<td>McGill University</td>
<td><a href="mailto:rustam.khalilullin@mcgill.ca">rustam.khalilullin@mcgill.ca</a></td>
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<tr>
<td>Viki Kumar Prasad</td>
<td>University of British Columbia, Okanagan</td>
<td><a href="mailto:vikikumarprasad@gmail.com">vikikumarprasad@gmail.com</a></td>
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<tr>
<td>Mathew Larade</td>
<td>University of Prince Edward Island</td>
<td><a href="mailto:m.c.larade@gmail.com">m.c.larade@gmail.com</a></td>
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<tr>
<td>Luc LeBlanc</td>
<td>Dalhousie University</td>
<td><a href="mailto:luc.leblanc@dal.ca">luc.leblanc@dal.ca</a></td>
</tr>
<tr>
<td>Zhe Li</td>
<td>Dalhousie University</td>
<td><a href="mailto:zheli@dal.ca">zheli@dal.ca</a></td>
</tr>
<tr>
<td>Bryan Linford</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:bdl207@mun.ca">bdl207@mun.ca</a></td>
</tr>
<tr>
<td>Csongor Matyas</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:cfm482@mun.ca">cfm482@mun.ca</a></td>
</tr>
<tr>
<td>Kelsey Menard</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:kjm408@mun.ca">kjm408@mun.ca</a></td>
</tr>
<tr>
<td>Mohamad Mohebifar</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:mmohbeifar@mun.ca">mmohbeifar@mun.ca</a></td>
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<td>Alastair Price</td>
<td>Dalhousie University</td>
<td><a href="mailto:a.price@dal.ca">a.price@dal.ca</a></td>
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<tr>
<td>Adam Proud</td>
<td>University of Prince Edward Island</td>
<td><a href="mailto:aproud@upei.ca">aproud@upei.ca</a></td>
</tr>
<tr>
<td>Jayendran Rasaiah</td>
<td>University of Maine</td>
<td><a href="mailto:rasaiah@maine.edu">rasaiah@maine.edu</a></td>
</tr>
<tr>
<td>Christopher Rowley</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:crowley@mun.ca">crowley@mun.ca</a></td>
</tr>
<tr>
<td>Fatemehsadiat Sajadi</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:fsajadi@mun.ca">fsajadi@mun.ca</a></td>
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<tr>
<td>Jeremy Schofield</td>
<td>University of Toronto</td>
<td><a href="mailto:jmschofi@chem.utoronto.ca">jmschofi@chem.utoronto.ca</a></td>
</tr>
<tr>
<td>Andrew Walsh</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:agw274@mun.ca">agw274@mun.ca</a></td>
</tr>
<tr>
<td>Evan Walters</td>
<td>Memorial University of Newfoundland</td>
<td><a href="mailto:etw148@mun.ca">etw148@mun.ca</a></td>
</tr>
<tr>
<td>Feng Xibo</td>
<td>Dalhousie University</td>
<td><a href="mailto:frederick.hillsfeng@dal.ca">frederick.hillsfeng@dal.ca</a></td>
</tr>
<tr>
<td>Tao Zeng</td>
<td>Carleton University</td>
<td><a href="mailto:toby.zeng@carleton.ca">toby.zeng@carleton.ca</a></td>
</tr>
<tr>
<td>Elias Zoghaib</td>
<td>Dalhousie University</td>
<td><a href="mailto:elias.zoghaib@dal.ca">elias.zoghaib@dal.ca</a></td>
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