

2020 JCP Emerging Investigator Special Collection

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INTRODUCTION

The Journal of Chemical Physics Emerging Investigator Special Collection and Best Paper Award were first launched in 2019 to recognize the achievements of early career researchers.^{1,2} In this editorial, we present the 2020 collection, a highly selective series describing the research supervised by principal investigators early in

their careers (10 years or less since Ph.D. graduation). The collection spans the scope of topics in chemical physics and physical chemistry and encourages contributed papers. Of the excellent papers published in the collection, two are chosen by a sub-committee of the Editorial Advisory Board as winners of the JCP Best Paper by an Emerging Investigator Award. The following are the 2020 winners:



Brianna R. Heazlewood,
EPSRC Early Career Fellow,
University of Liverpool, UK

[“A stand-alone magnetic guide for producing tuneable radical beams,”](#)²¹

Chloé Miossec, Lok Yiu Wu, Paul Bertier, Michal Hejduk, Jutta Toscano, and Brianna R. Heazlewood



Stephen J. Cox,
Royal Society University Research Fellow,
University of Cambridge, UK,
Photo Credit: University of Cambridge

[“Macroscopic surface charges from microscopic simulations,”](#)³⁵

Thomas Sayer and Stephen J. Cox

The 2020 collection comprises 36 impressive contributions. As a service to the community, the JCP editors who handled the papers included in the 2020 collection have summarized them and highlighted their significance below, organized by the Journal's Table of Contents sections.

THEORETICAL METHODS AND ALGORITHMS

The Theoretical Methods and Algorithms section is well represented in the present collection, with a total of 14 papers. These papers span the full range of theoretical and computational methodology of relevance to chemical physics, from advances in electronic structure theory to developments in biomolecular simulation.

Several papers report developments in electronic structure theory and density functional theory (DFT), including two separate papers on excited states. The GW method is widely used to compute excitation energies in periodic systems. However, most formulations to date are either computationally costly or involve approximations to the frequency-dependent self-energy. In their Communication, Bintrim and Berkelbach show how to simultaneously decrease computational cost and formulate the method without frequency dependence.³ This work could open the door to more accurate and more routine calculations of excited states in materials such as photovoltaics. In their article, Hardikar and Neuscamm show how to treat excited states with a Hartree–Fock like self-consistent field approach.⁴ This could provide an efficient new starting point for computing excited electronic states of gas phase molecules.

Herbst and Fransson consider the core-valence separation approximation that is often used in the calculation of core-level spectra.⁵ They show how to quantify the errors in this approximation, thereby opening the door to error-quantified predictions relevant to x-ray spectroscopy. Brémond *et al.* show that a simple approach to determining the range-separation parameter in hybrid and double hybrid density functionals can provide accurate ionization potentials.⁶ The parameter is chosen to recover the total energy of the hydrogen atom and offers an efficient alternative to optimal tuning procedures. Tovi and Caspary Toroker use wavefunctions propagated on DFT potential energy surfaces to study charge-transport across interfaces.⁷ Their two-dimensional model is applied to charge-transport at metal/metal oxide interfaces and shown to allow for more transport pathways than the one-dimensional model that has previously been used. Marom and co-workers describe a new software package for generating molecular crystal surfaces, calculating surface energies, and predicting crystal shapes using DFT.⁸ This code will be useful for researchers interested in pharmaceuticals, organic semiconductors, and certain energy materials. We would welcome the submission of further papers describing chemical physics computer codes for publication in the new Chemical Physics Software section of JCP.⁹

Machine learning is assuming an increasing importance in chemical physics, not least in the context of constructing electronic potential energy surfaces. The present collection contains two separate papers in this area. In his paper on mean-field density matrix decompositions, Eriksen uses localized orbitals and energy

partitioning to create a set of features for machine learned representations of molecular potential energy functions.¹⁰ These features could lead to more accurate and more easily learned neural network potentials. Jiang and co-workers show how active learning techniques can be used to provide accurate approximations of reactive potential energy surfaces from neural networks.¹¹ They also show how the error in these neural network potentials can be quantified. This strategy is a promising approach for obtaining accurate potential energy surfaces suitable for use with quantum dynamics methods.

The collection also contains two contributions on modern aspects of quantum dynamics. Chiang and Hsu use the driven Liouville-von Neumann approach to account phenomenologically for electronic relaxation in the electrodes in quantum transport across model tunneling systems.¹² They assess the effect of the relaxation on the steady state current by comparing their results to the Landauer formula. Herrera and co-workers extend their work on vibrational polaritons, which was also featured in the Emerging Investigator Special Topic Collection last year.¹³ In the present contribution, they show how coupling a quantized infrared cavity field to an anharmonic molecular vibration affects both the molecular bond length and the number of excited cavity photons. Applications to ground electronic state HF and CO₂ molecules are used to illustrate their predictions.

Path integral methods provide a well-established way to include quantum effects in the nuclear motion in condensed phase simulations. However, it is far less common to see these methods applied to electrons. The present collection contains two separate contributions in this area. In their Communication, Remsing and Bates report an ingenious combination of effective mass theory and path integral molecular dynamics for studying the interactions of electrons with condensed phase environments.¹⁴ Their methodology allows for the anisotropy of the electronic band structure in determining the effective mass tensor, which enables its application to anisotropic materials. Applications to an exciton in solid KCl and electron trapping by a sulfur vacancy in monolayer MoS₂ nicely illustrate the utility of the approach. Hirshberg and co-workers use the Bogoliubov inequality to alleviate the fermionic sign problem in path integral Monte Carlo simulations.¹⁵ They demonstrate that this approach leads to a significant speed-up in example applications to up to six spin-polarized electrons confined in harmonic traps. The fermionic sign problem is notoriously difficult, and this work does not provide a complete solution to it, but the idea is interesting, and the results presented in the manuscript are encouraging for further applications to few-fermion systems.

There has been considerable recent interest in the development of algorithms for non-equilibrium statistical mechanics, and this too is reflected in the present collection. Das and Limmer develop a novel algorithm to address the inverse problem of the optimal design of targeted, self-assembled colloidal clusters under non-equilibrium steady-state conditions.¹⁶ They find that clusters can be formed in high yield with specific short ranged interactions of varying complexity. Hussain and Haji-Akbari use accurate calculations of heterogeneous ice nucleation rates on model surfaces to understand the role of finite size effects in nucleation simulations.¹⁷ Their work addresses an important and often ignored issue in the simulation of nucleation from solution. Albaugh and Gingrich explore strategies to efficiently compute variations in reaction rates over a

chemical design space, which might be defined in terms of varying particle charges, residue identities, or force field parameters, using transition path sampling.¹⁸ They demonstrate the validity of their approach through applications involving two toy model systems for which the rates depend on model parameters defining the design.

The collection also contains two interesting papers on biomolecular simulation. A grand challenge in molecular biophysics is to observe the dynamical motions of biomolecules with atomistic resolution. Topel and Ferguson address this challenge by exploiting the embedding theory of Takens and integrating techniques from statistical thermodynamics, artificial neural networks, and rigid graph theory to develop a trained model to predictively reconstruct atomistic molecular configurations from time series data.¹⁹ Through applications to a polyethylene chain and a small protein, the authors demonstrate the ability to accurately reconstruct the molecular configuration of a macromolecule from the time series in a single experimental observable. Another biophysical modeling paper by Jiang and Wang provides the first transition charge coupling model for C=O and C=C vibrations of nucleobases in which the interactions of the chromophores reflect the three-dimensional structures of nucleic acids.²⁰ This theoretical framework provides a bridge between molecular dynamics simulations and vibrational spectroscopy experiments. It should therefore be useful in both facilitating the interpretation of spectra and guiding the design of new experiments.

ADVANCED EXPERIMENTAL TECHNIQUES

Preparing well-controlled beams of free radicals for chemical reactions has been a challenge, owing to the difficulties associated with generating and selecting radical species. In their article, Heazlewood and co-workers report a novel and versatile guide that produces a pure, state-selected, tunable beam of hydrogen atoms simply using permanent magnets.²¹ This device with further development will make it possible to study a range of chemical reactions with radical species free from competing side reactions and with a high degree of control over the properties of the radical reactants. Brianna Heazlewood received one of the two “Best Paper by an Emerging Investigator” awards for this paper.

Oxide clusters are important model systems for catalysts and therefore an interesting target for spectroscopic investigation. In their Communication, van der Linde and co-workers were able to characterize the fundamental vibrational properties of the three small transition metal oxide cations MO₂⁺ (M = V, Nb, and Ta) using multiphoton infrared dissociation spectroscopy in an ion cyclotron resonance mass spectrometer.²²

Intracellular water is critical for cellular function, yet methods for direct visualization of subcellular solvation are lacking. Lang and Welsher present a new imaging approach that combines spectral-focusing hyperspectral stimulated Raman scattering with an environmentally sensitive nitrile probe.²³ They demonstrate their method in the solution phase, microscopic droplets, and cellular environments, showing the promise of their approach for mapping heterogeneous solvation in complex systems with high spatiotemporal resolution.

ATOMS, MOLECULES, AND CLUSTERS

Particle formation in the atmosphere is a complicated process. The study by Johnson and co-workers aims to elucidate the

role of water in new particle formation using well-defined hydrated ammonium bisulfate clusters as models.²⁴ Using a temperature-controlled ion trap and infrared spectroscopy, the authors were able to isolate structural motifs of hydrated ammonium bisulfate clusters and study their thermal stability.

PAHs (polycyclic aromatic hydrocarbons) are ubiquitous in the interstellar medium (ISM), so understanding their photophysics and photochemistry is important in astrochemistry. Stockett *et al.* report quantitative data concerning the unimolecular fragmentation and electronic and vibrational relaxations of ionized perylene, which will be valuable for understanding the fate of PAHs in the ISM.²⁵

Competing quantum effects in hydrogen bonding systems were first identified over a decade ago and have since been discussed in numerous papers published in JCP. In their contribution, Zhou and Wang report an *ab initio* path integral molecular dynamics study of the bifurcated short hydrogen bond in TAPH (see their paper for an expansion of the acronym), which exhibits a significantly elongated N–H bond length and a downfield ¹H nuclear magnetic resonance (NMR) chemical shift of 22.1 ppm.²⁶ The properties of this hydrogen bond are contrasted with those of the linear short hydrogen bond in DMANH (ditto). Competing nuclear quantum effects are identified in an analysis of the simulations, and the calculations are shown to yield excellent agreement with experiment for the ¹H NMR chemical shift. Overall, the study sheds considerable new light on the nature of short intramolecular hydrogen bonds in solution.

There is a wide literature on the impact of molecular vibrations in mediating spin-state switching in transition metal complexes, but little connection has been made between this literature and the understanding of vibrations in molecular qubits, or to traditional inorganic chemistry concepts such as zero-field splittings. In their paper, Hadt and co-workers use a combination of analytical ligand field theory and high-level *ab initio* calculations to bridge these gaps.²⁷ Their identification of the excited state coupling terms that help to mediate intersystem crossing is of particular interest, as it may aid the design of new spin crossover materials.

LIQUIDS, GLASSES, AND CRYSTALS

The study of freezing in two dimensional systems has been a problem of interest since the 1950s. In their paper, Sampedro Ruiz and Ni study the freezing of mixtures of hard disks.²⁸ In particular, they consider polydisperse systems with different distributions. They analyze the types of phase transitions between fluid, hexatic, and solid phases depending on the polydispersity for several distributions (Gaussian, log, and triangular). For the Gaussian and log distributions, some evidence is found of a continuous transition between the fluid and the hexatic phase at high polydispersities. However, in the triangular distribution, the fluid-hexatic transition appears always to be first order. The study illustrates how the particle size distribution is of primary importance in determining the phase behavior of polydisperse hard disks.

Water has two amorphous glassy phases, one with a low density denoted LDA and another with high density denoted HDA. Using long computer simulations of the tip4p/2005 water model, Martelli *et al.* are able to show that both the LDA and HDA amorphous phases are genuine glassy states, which have an equilibrium counterpart at the thermodynamic conditions accessible to computer simulations.²⁹ Using neural networks, the structural similarity between the glassy phases and the structures found in the equilibrated

liquid is demonstrated. The calculations also show critical fluctuations in density in the proximity of the critical point of the model, with a large amount of LDA water when the density is low, and of HDA and high-T water when the density is high. This work clarifies the structural connection between the non-equilibrium and the equilibrium phase diagrams of water.

MATERIALS, SURFACES, AND INTERFACES

Hot electron transfer at material interfaces is usually hard to quantify. Zhu and co-workers tackle this problem for a model system containing a 2D semiconductor heterojunction and show convincingly the efficient hot electron transfer from photoexcited MoTe₂ to WS₂.³⁰ This finding provides important insight into the competition between hot electron cooling and transfer at 2D semiconductor interfaces and suggests an intriguing possibility for the exploration of hot electron devices.

Atomically precise fabrication of nanostructures has the potential for developing new materials for a wide range of applications. Jiang and co-workers use high resolution STM to investigate the reaction and self-assembly of (3,6-dibromo-9,10-phenanthrenequinone, or DBPQ) molecules on Ag (100) and Ag (110) surfaces in order to understand the mechanism of bottom-up assembly on surfaces.³¹ They show that, through the inclusion of multiple functional groups within a precursor molecule, it becomes possible to fabricate new low-dimensional materials with unique chemical, physical, and electronic properties.

Chen *et al.* report an *ab initio* study of titanium dioxide that accomplishes a remarkable technical feat.³² They use embedding approaches to study the electronic state of an oxygen vacancy in TiO₂ at high levels of quantum chemistry, validating with full configuration interaction quantum Monte Carlo (FCIQMC) as well as coupled cluster theory with single, double, and perturbative triple excitations [CCSD(T)] the singlet nature of the ground state. The results are relevant for the characterization of defects in TiO₂ and more broadly demonstrate how to apply gold-standard quantum chemistry methods to the condensed phase.

The toxicity of lead and the material instability of lead-halide perovskites have led to the search for alternative materials for photovoltaic devices. In their Communication, Chen and co-workers report a DFT study of a range of lead-free perovskites.³³ Their focus is on Cs₂MBiCl₆ materials, with M corresponding to a variety of different metals. Interesting periodic trends in the electronic properties and crystal structures are identified and analyzed.

Gattinoni and co-workers provide an original perspective and a fresh understanding of the surface properties of ferroelectrics, in terms of “surface happiness”—a concept that loosely reflects the compensation of surface charge and polarization.³⁴ The interplay between surface charge, polarity, and defects has technologically relevant implications for the manufacture of devices incorporating ferroelectric components, and for the use of these materials for catalysis.

Charged surfaces in contact with solution are commonplace in fields as diverse as colloid science, geology, and energy materials. However, performing computer simulations of these systems is fraught with difficulties. Sayer and Cox show how commonly used simulation approaches lead to qualitatively incorrect descriptions of

ion adsorption at charged interfaces.³⁵ They propose a new methodology, inspired by an earlier method of Sprik and co-workers, that provides the correct description of the interface between NaCl and its solution. Their methodology can be incorporated easily in existing simulation packages, and it is hoped that the results presented will be useful to the simulation community in modeling charged solid/liquid interfaces. Stephen Cox received one of the two “Best Paper by an Emerging Investigator” awards for this paper.

POLYMERS AND SOFT MATTER

Microphase separation of block copolymers is an intriguing topic, and the understanding of copolymer phase behaviors has important implications in materials design and functional applications. In their contribution, Li and Liu systematically investigate the general phase behavior of a class of miktoarm star copolymers using self-consistent field theory, revealing the connection between the phase behavior in the strong-segregation regime and the overall phase diagram topology.³⁶ This study provides insights into the phase behaviors of copolymer systems with complicated chain architectures and conformational properties.

Programmable self-assembly is a promising strategy for making ensembles of nanostructures from synthetic components, but one that is often thwarted by a lack of predictability. The paper by Rogers addresses a significant challenge faced in directing the assembly of complex molecular structures.³⁷ The author advances the concept of encoding assembly instructions in molecules dispersed in solution, rather than molecules on particle surfaces. He shows that this leads to new phase behavior which could represent an advance toward the goal of programmable self-assembly.

BIOLOGICAL MOLECULES AND NETWORKS

The inherently stochastic oscillations that govern the function of biochemical clocks can be modeled using analytically tractable Markov state models. In their paper on this topic, del Junco and Vaikuntanathan present new analytical results that extend the analysis of Markov state models to networks consisting of a large cycle decorated with multiple small cycles.³⁸ An interesting implication of their analysis is that, for a high “energy budget,” different network topologies can become degenerate in terms of the period of oscillations. This suggests that biochemical oscillators can be more robust to fluctuations when they have a high energy budget.

In allosteric signal propagation involving membrane proteins, stimuli often act at a site distant from the effector site. In their Communication, Delemotte and co-workers expand the network approach, often used to analyze allosteric mechanism, to include lipid membrane and other co-factors in the analysis of three membrane protein systems.³⁹ Importantly, they observe that the binding of specific small molecules may act to rewire the network and influence the role of lipids in allosteric signal propagation.

2021 COLLECTION AND AWARDS

The 2021 Emerging Investigator Collection is open for submissions and already publishing. The deadline for acceptance into the 2021 collection is December 31, 2021. Papers accepted after that date will be included in the 2022 collection and considered for the 2022 awards. For more information, please see

the journal website: <https://aip.scitation.org/jcp/info/awards>. To go directly to how to submit and eligibility requirements, please see the call for paper page: <https://publishing.aip.org/publications/journals/special-topics/jcp/2021-jcp-emerging-investigators-special-collection/>.

We look forward to many more annual collections recognizing early career researchers. If you have any questions or comments, please contact us at jcp-journalmanager@aip.org.

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