VISTA Seminar

Seminar 43

October 19, 2022

10:00 am – 11:30 am EDT / 3:00 – 4:30 BST / 4:00 pm – 5:30 pm Paris

TOC:

Incorporating Nuclear Quantum Effects in *ab initio* Molecular Dynamics for Accurate and Efficient Vibrational Spectra Calculations

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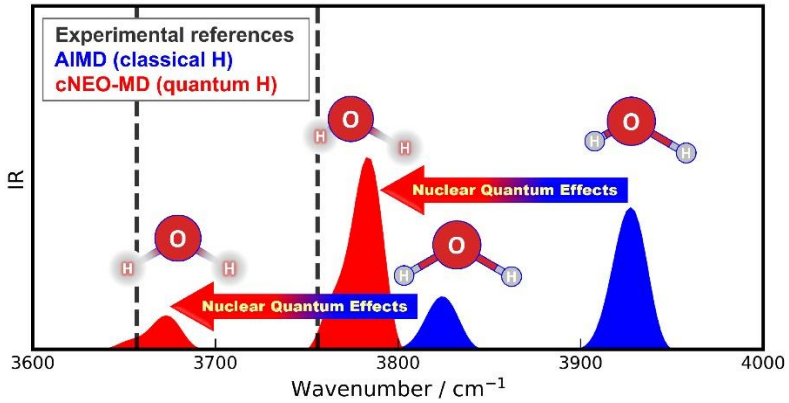

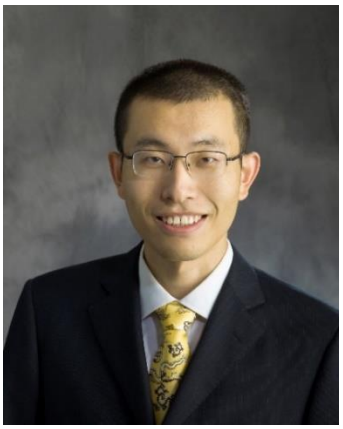

Nuclear quantum effects play a significant role in a variety of chemical and biological processes, but it remains challenging to accurately include them in large-scale molecular simulations. Recently, we developed a new molecular dynamics method named constrained nuclear−electronic orbital molecular dynamics (CNEO-MD) for the accurate and efficient incorporation of nuclear quantum effects in molecular simulations. This new MD approach is a combination of our previously developed constrained nuclear−electronic orbital density functional theory (CNEO-DFT) and constrained minimized energy surface molecular dynamics (CMES-MD). We employed CNEO-MD to calculate the vibrational spectra of a series of molecules and the results are compared to those from conventional *ab initio* molecular dynamics (AIMD) as well as from experiments. With the same formal computational scaling, CNEO-MD greatly outperforms conventional AIMD, especially for the vibrational modes with significant hydrogen motion characters. This development provides an accurate and efficient method for calculating vibrational spectra for systems involving hydrogen atoms, which are ubiquitous in chemistry and biology. Additionally, the applications of CNEO-MD to the study of other static and dynamic properties are also under investigation in our group.

Charge-Transfer Landscape Manifesting the Structure–Rate Relationship in the Condensed Phase *Via* Machine Learning

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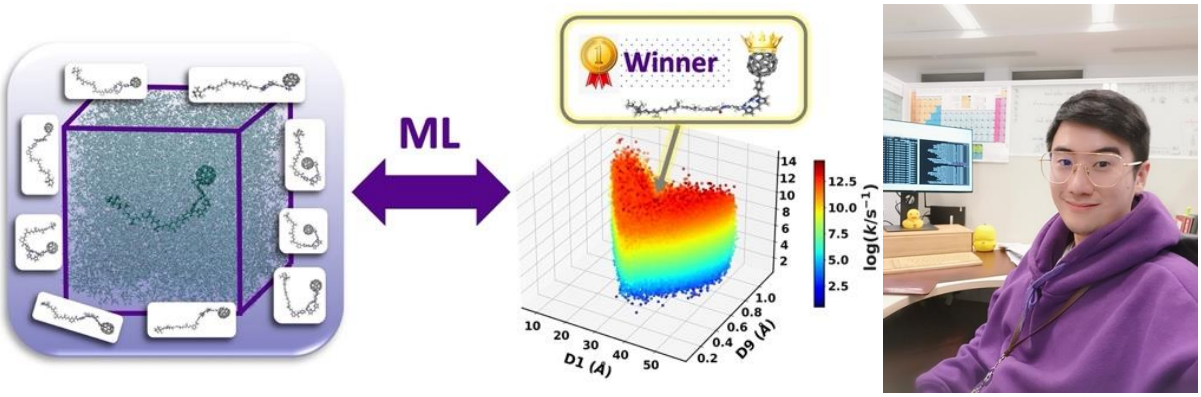

Understanding and designing high-efficiency organic photovoltaics (OPV) material that, at the same time, is solution-processable offers promise for scalable and economical OPV devices toward large-scale renewable energy production, accelerating the global energy transition. To this end, molecular insights into the underlying conformation-dependent charge transfer properties in the condensed phase are crucial. In this work, we develop a simulation strategy aided by machine learning (ML) to map the molecular structure to condensed phase charge-transfer (CT) properties. The properties include CT rate constants, energy levels, electronic couplings, energy gaps, reorganization energies, and reaction-free energies, which are called CT fingerprints. The ML models exhibit high predictive power and error within chemical accuracy, empowering the construction of CT landscape for millions of molecular dynamics sampled structures and allowing for instant prediction of CT rate properties taking molecular structures as input. We demonstrate some immediate utilities of the CT landscape for calculating the ensemble-averaged CT rate constant and interpreting the correlation effects of molecular structural features on the CT rate. We foresee the CT landscape will be useful for investigating real-time CT dynamics in nanoscale- and mesoscale-condensed phase systems and for optimal fabrication design of molecules facilitated by a reverse search based on target CT properties criteria.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 43
Time: Oct 19, 2022 10:00 AM Eastern Time (US and Canada)

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