VISTA Seminar

Seminar 17

April 28, 2021

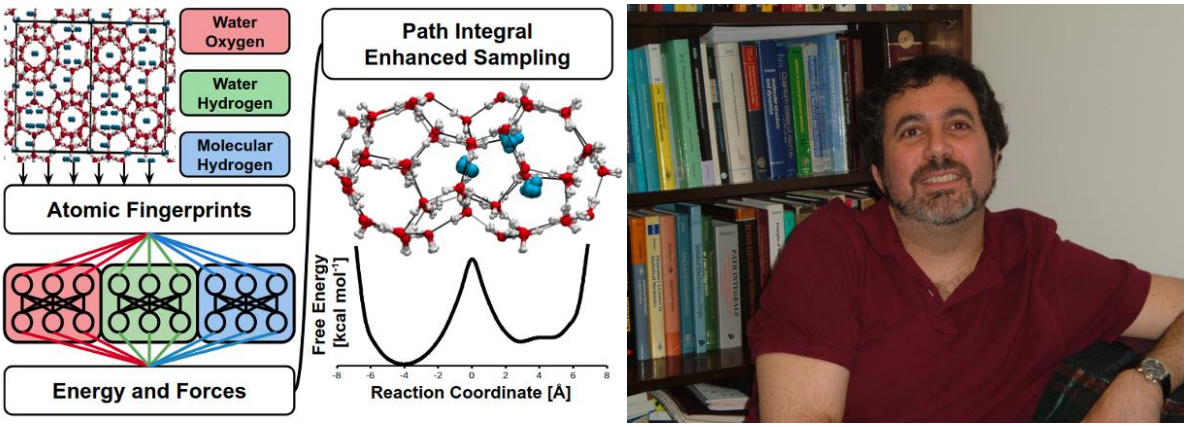
9:30 – 11:00 am EDT / 1:30 – 3:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

Combining path integral molecular dynamics with machine learning potentials for the study of complex quantum phenomena in condensed phases

Mark E. Tuckerman

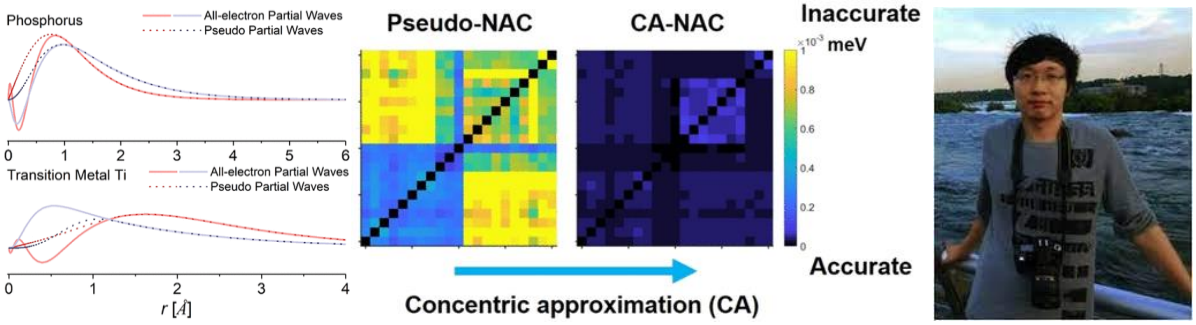
Department of Chemistry, New York University, 100 Washington Square East, New York, NY 10003
Courant Institute of Mathematical Sciences, New York University, 251 Mercer St. New York, NY 10012
NYU-ECNU Center for Computational Chemistry at NYU Shanghai, 3663 Zhongshan Rd. N. Shanghai 200062 People's Republic of China
Email: mark.tuckerman@nyu.edu



Reliable simulation of complex chemical processes in condensed phases requires an accurate quantum mechanical description of the interatomic interactions in the system. If these are to be used in a molecular dynamics calculation, they are often generated "on the fly" as the simulation proceeds, a technique known as *ab initio* molecular dynamics (AIMD). Given the high computational cost of these calculations, alternative approaches employing machine learning methods represent an attractive alternative and have become increasingly popular. As the adoption of machine-learning potential becomes more widespread, it is important to consider how simulations employing them should be carried out. Specifically, as they do not implicitly include nuclear quantum effects, these effects must be included explicitly, and the most efficient way to do this is via the use of Feynman path integral techniques. In this talk, I will discuss the combination of machine learning of potentials, path-integral molecular dynamics and enhanced sampling methods for treating molecular hydrogen diffusion in structure-II clathrate as an example of a problem that requires this synergy of approaches. I will also discuss different approximation schemes for obtaining dynamical properties within the path-integral framework.

How to calculate Non-adiabatic Coupling Accurately and Efficiently

Weibin Chu, Oleg V. Prezhdo
University of Southern California, Department of Chemistry, Los Angeles, California 90089, United States
Email: wc_086@usc.edu



Non-adiabatic (NA) molecular dynamics (MD) simulation is a popular and versatile method that reached great success. However, the accurate computation of NA coupling, a crucial quantity in those simulations, is the key prerequisite. NAMD in solid, surface, and interface is often implemented with the projector augmented-wave (PAW) method, which provides a convenient representation of the all-electron (AE) wavefunction and relates it to the pseudo (PS) wavefunction by a linear transformation. NAC calculated with AE wavefunctions requires integration between the atom-centered radical and plane waves grids, which is rather complicated and computationally expensive. Therefore, the calculation of NAC with PS wavefunctions has become a popular alternative without a rigorous validation for a long time. **However, PS wavefunctions are neither eigen-wavefunctions nor orthogonal wavefunctions.** In our exhaustive evaluation, **we found NAC calculated with PS wavefunctions will cause large errors in system with transition metal.**[1] Here, we introduced a generalized method employing concentric approximation (CA) for accurate and efficient NAC calculation with PAW pseudopotential.[2] Our proposed CA NAC **reduces the error more than an order of magnitude** over the widely used PS NAC, making the accuracy comparable to the exact AE NAC. At the same time, **the computational cost of the CA NAC evaluation is 3-4 orders of magnitude lower** than the evaluation of the exact AE NAC.

1. Chu, Zheng, Akimov, Zhao, Saidi, Prezhdo: Accurate Computation of Non-adiabatic Coupling with Projector Augmented-Wave Pseudopotentials. *J. Phys. Chem. Lett.*, **11** (2020), 10073-10080.
2. Chu, Prezhdo: Concentric Approximation for Fast and Accurate Numerical Evaluation of Non-adiabatic Coupling with Projector Augmented-Wave Pseudopotentials. *J. Phys. Chem. Lett.*, **12** (2021), 3082-3089.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 17
Time: Apr 28, 2021 09:30 AM Eastern Time (US and Canada)

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