VISTA Seminar

Seminar 71

June 12, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

First-Principles Approach to Coupled Quantum Dynamics of Electrons and Protons in Heterogeneous Systems

Yosuke Kanai

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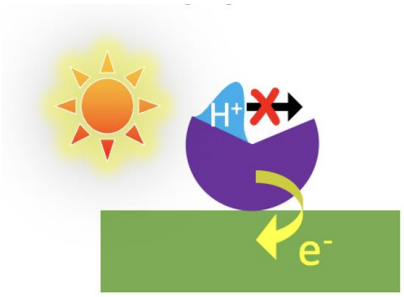

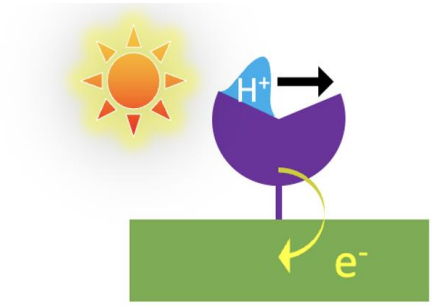

The coupled quantum dynamics of electrons and protons is ubiquitous in many dynamical processes involving light-matter interaction, such as solar energy conversion in chemical systems and photosynthesis. A first-principles description of such nuclear-electronic quantum dynamics requires not only the time-dependent treatment of nonequilibrium electron dynamics but also that of quantum protons. We discuss the new real-time nuclear-electronic orbital time-dependent density functional theory (RT-NEO-TDDFT) approach to study such dynamics in complex extended systems. We apply the new first-principles method to studying coupled quantum dynamics of electrons and protons in complex heterogeneous systems for its crucial role in photochemical catalytic reactions pursued in the Department of Energy (DOE) Energy Innovation Hub, Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE). In particular, we investigate electronically excited state intramolecular proton transfer in water and at semiconductor-molecule interface. The calculations illustrate how environments such as hydrogen-bonding water molecules and an extended material surface impact the dynamical process on the atomistic level. I will conclude by discussing outstanding challenges and other related development from my research group at UNC.

Towards efficient excited state calculation at extreme conditions with mixed deterministic-stochastic hybrid exchange.

Joshua A. Leveillee

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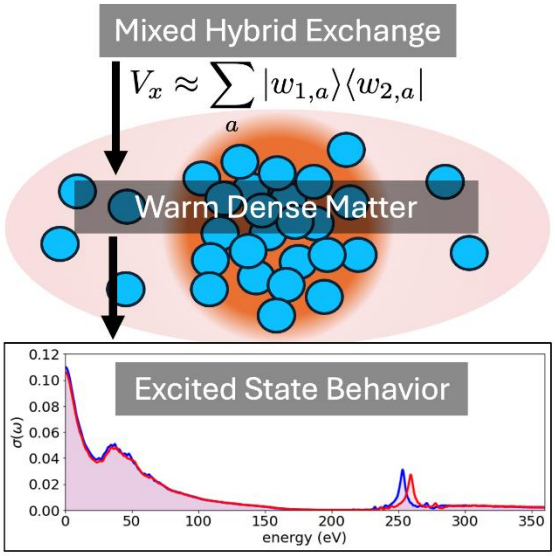

Predicting the electronic structure of matter under extreme conditions, such as warm dense matter and hot dense plasmas, is a challenging undertaking. Modern methods of mixing deterministic and stochastic density functional theory (mDFT) have resulted in excellent scaling of efficiency with temperature to determine the finite temperature equilibrium states. Excited state calculations are a natural next step to which we may apply these methods. In this talk, I will review the background of mDFT and discuss our recently developed method of mixed deterministic-stochastic electronic hybrid exchange to determine the electronic structure of warm dense matter. We additionally develop a novel compression scheme for the mixed exchange operator to accelerate calculations at high temperature. We find that including hybrid exchange influences the predicted energies of electronic states even up to extreme temperature (T > 20 ev) and strongly influences predicted deep ultra-violet / soft x-ray AC conductivities of warm dense neon gas and beryllium metal.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 71
Time: Jun 12, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/93906726060?pwd=bmdAiUMWC0Egeza2UlP8HighR2stb2.1

Meeting ID: 939 0672 6060
Passcode: 043831