VISTA Seminar

Seminar 42

October 5, 2022

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

TOC:

Cracking Challenging Electronic Structures: Embedding, machine learning and orbital-free DFT are the key

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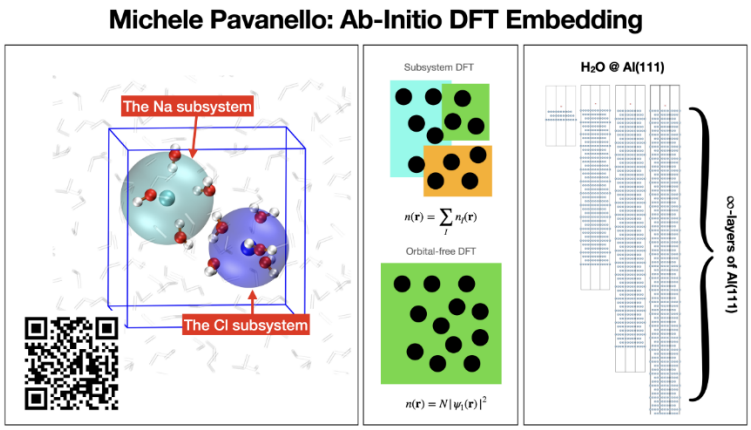

Challenging electronic structures are of two types: (1) Large systems, too large for conventional electronic structure methods, (2) Strongly correlated electrons, where a mean-field treatment of the electronic systems is inadequate. In this talk I will show that a combination of embedding, orbital-free DFT, Kohn-Sham (KS)-DFT and machine learning successfully tackles both challenges for such systems as molecular condensed phases and interfaces of sizes untouchable by mainstream methods. My talk will focus on nonstandard embedding workflows of recent formulation. These include embedding KS-DFT subsystems in orbital-free DFT for the improved treatment of interfaces involving metallic systems. We also developed a machine learning (ML) method where the learned quantity is the one-electron reduced density matrix. Exploiting the theorems of reduced density matrix functional theory, we learn KS-DFT as well as post-Hartree-Fock methods delivering accurate predicted electronic structures, energies and forces for ab-initio molecular dynamics simulations in record wall-times. To make the methods available to the broader community, in the past 3 years we produced Python implementations of electronic structure solvers in plane wave basis based on Quantum ESPRESSO (QEpy) as well as ML-based solvers (QMLearn), orbital-free DFT (DFTpy) and density embedding (eDFTpy). With this arsenal at our disposal, we are ready to tackle the most difficult and timely electronic structure challenges.

Floquet nonadiabatic dynamics: electron and energy transfer driven by light-matter interactions

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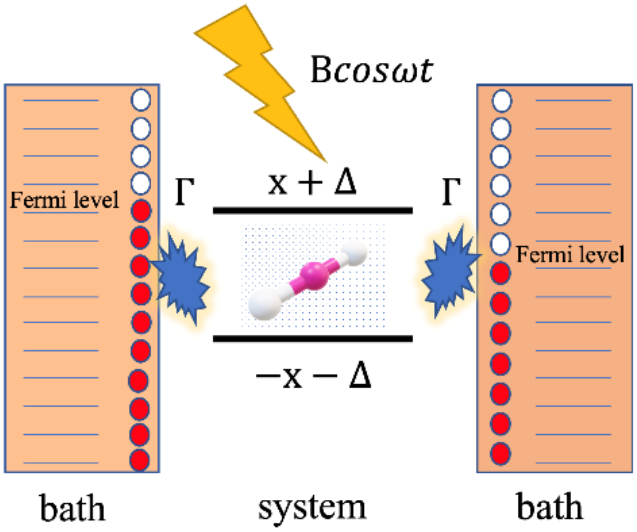

Strong light-matter interactions on metallic surfaces are highly relevant for various chemical systems, including photoinduced chemical adsorption, photoelectrical catalysis and polariton chemistry. However, such systems are challenging for theoretical study: the Born-Oppenheimer (BO) approximation fails to describe the nonadiabatic dynamics at metal surfaces, and the perturbation theory is no longer valid for strong light-matter interactions. Here, we have derived a Floquet electronic friction approach to describe the nonadiabatic dynamics near metal surfaces subjected to periodic light driving, and such friction can be recast into a form in terms of Green's functions. We demonstrated that the frictional tensor shows antisymmetric Lorenz-like force even without bias. We further benchmarked our Floquet electronic friction dynamics against the Floquet surface hopping approach for one-level resonant systems near metal surfaces. We found that the strong light-matter interaction can strenuously affect the electron transfer rate near surfaces.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 42
Time: Oct 5, 2022 10:00 AM Eastern Time (US and Canada)

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