

VISTA Seminar

Seminar 48

February 15, 2023

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT London / 4:00 pm –
5:30 pm CET Paris / 11 pm CST Beijing**

TOC:

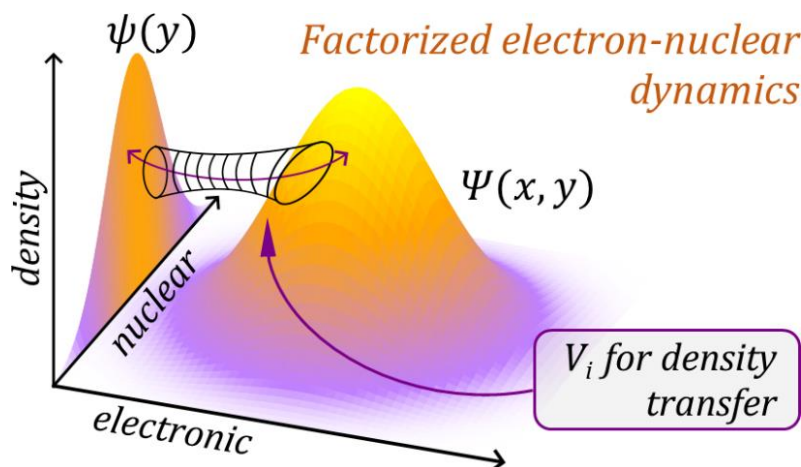
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Factorized Electron-Nuclear Dynamics with an Effective Complex Potential

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We present a quantum dynamics approach for molecular systems based on wavefunction factorization into components describing the light and heavy particles, such as electrons and nuclei. The dynamics of the nuclear subsystem can be viewed as motion of the trajectories defined in the nuclear subspace, evolving according to the average nuclear momentum of the full wavefunction. The probability density flow between the nuclear and electronic subsystems is facilitated by the imaginary potential, derived to ensure a physically meaningful normalization of the electronic wavefunction for each configuration of the nuclei, and conservation of the probability density associated with each trajectory in the Lagrangian frame of reference.

An effective real potential, driving the dynamics of the nuclear subsystem, is defined to minimize motion of the electronic wavefunction in the nuclear degrees of freedom.

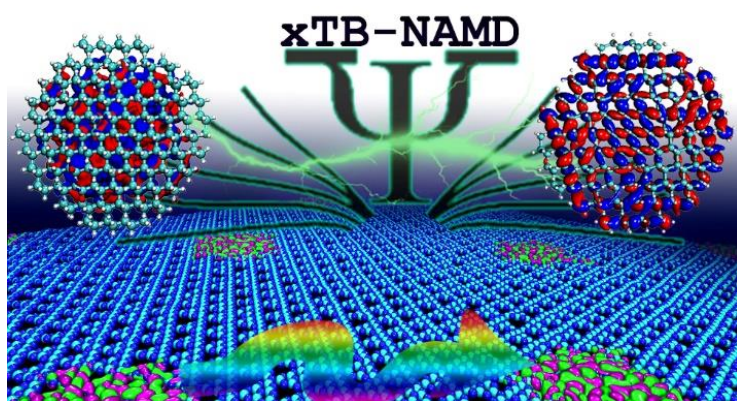
Illustration and the analysis of the formalism are given for a two-dimensional model system of vibrationally nonadiabatic dynamics.

Nonadiabatic molecular dynamics simulations in large scale nanomaterials and periodic solids

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Nonadiabatic molecular dynamics (NA-MD) simulations provide valuable atomistic insights into the photoexcitation dynamics in solar energy materials. Such simulations have been utilized in the photoexcited dynamics of different materials with applications in solar cells, light-emitting diodes, photocatalysis, etc. However, modeling such simulations for structures with sizes close to those observed in experimental studies are computationally expensive and the simulations are limited to small- and medium-sized structures with few hundreds of atoms.

For larger structures, usually semiempirical and density functional tight-binding approaches are utilized. However, the parametrization are available only for some elements in the periodic table. The extended tight-binding (xTB) approach provides the parametrization for a wide range of elements including those present in inorganic materials such as quantum dots. This method can be applied to compute the electronic structure properties of large structures with thousands of atoms including metal organic frameworks and biological structures such as proteins. Therefore, this method can be used as a suitable tool in NA-MD simulations for large structures. Due to close energy levels spacing in large structures, one requires to include hundreds or thousands of electronic states to capture the excitation energies close to that observed in experiments and computation of the time-overlap integrals is a challenge.

In this presentation, I will highlight our most recent work on NA-MD simulations in the xTB framework. I will first talk about the implementation details, as is implemented in the open-source Libra code. Then, I will show the applicability of this approach for describing hot-electron relaxation dynamics in large silicon quantum dots. I will also talk about the dependence of the electron-hole recombination dynamics on charge carrier concentration in carbon nitride monolayers with up to 5600 atoms, that constitute supercells as large as 14.2 nm x 12.3 nm, approaching the nanoscale regime of experimental studies.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 48

Time: Feb 15, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/98833570449?pwd=T3lQnd3MXI4c0hVUINwdThXRkM3QT09>

Meeting ID: 988 3357 0449

Passcode: 406986