VISTA Seminar

Seminar 54

July 5, 2023

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

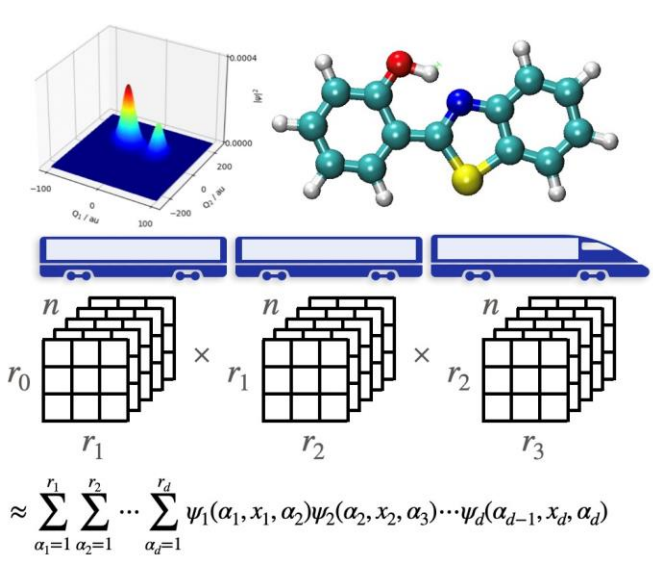
TOC:

Tensor-trains for highly multidimensional dynamics simulations

Micheline B. Soley

Department of Chemistry, University of Wisconsin-Madison, Wi, USA

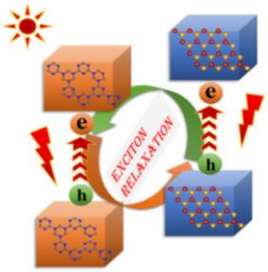
Email: micheline.soley@wisc.edu

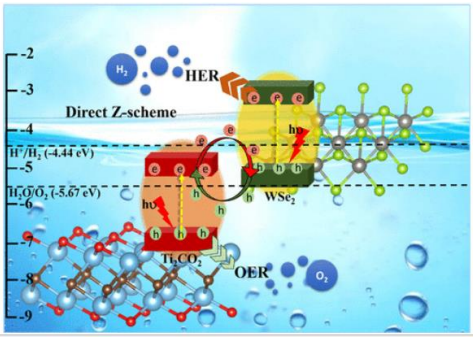


Quantum dynamics faces the "curse of dimensionality," in which the computational cost grows exponentially as the dimensionality increases. This curse frequently limits exact grid-based quantum dynamics simulations to molecular systems of no more than four atoms. In this talk, I will demonstrate the ability of data compression tensor-train techniques to surmount this curse and enable quantum dynamics in high dimensionality. I will introduce tensor-train Chebyshev (TT-Chebyshev) quantum dynamics, which makes possible simulation of molecular motions in up to 50D, and the tensor-train split-operator Fourier transform (TT-SOFT) method, which enables prediction of pump-probe spectra with full inclusion of quantum effects in ab initio potentials in up to 69D. To conclude, the talk will discuss the tensor-train Iterative Power Algorithm (IPA) for optimization of molecular potential energy surfaces and demonstrate how adaptation of method to quantum computers surpasses one of the foremost quantum computing approaches.

Rational Design of van-der Waals Heterostructures as Potential Photovoltaics and Photocatalysts: An Approach from Non-adiabatic Study

Atish Ghosh
Department of Chemistry, Visva-Bharati University, Santiniketan - 731235, India
Email: atishghosh.rs@visva-bharati.ac.in





Using density functional theory coupled with non-adiabatic molecular dynamics methodology, researchers have opened a new dimension that provides a precise theoretical understanding of efficient photovoltaic or photocatalytic activity.

In search of an efficient solar energy harvester, we herein performed a time-dependent density functional study to gain atomistic insight into the charge carrier dynamics of a graphitic carbon nitride (g-CN)–tungsten telluride (WTe_2) van-der Waals heterostructure. Our study predicted ultrafast electron (589 fs) and hole-transfer (807 fs) dynamics in g-CN/WTe_2 heterostructure and a delayed electron–hole recombination process (2.404 ns) as compared to that of the individual g-CN (3 ps) and WTe_2 (0.55 ps) monolayer. The ultrafast charge transfer is due to strong electron–phonon coupling during the charge-transfer process, while comparatively weak electron–phonon coupling, sufficient band gap, comparatively lower nonadiabatic coupling (NAC), and fast decoherence time slow down the electron–hole recombination process. The NAMD results of exciton relaxation dynamics are valuable for the insightful understanding of charge carrier dynamics and in designing photovoltaic devices based on organic–inorganic 2D van der Waals heterostructures.

One of the potential strategies to solve the renewable energy shortage is to design low-cost, efficient photocatalysts for water splitting to aid hydrogen and oxygen evolution reactions (HER and OER). Two-dimensional (2D) materials like MXenes and transition metal dichalcogenides (TMDs) have caught special attention owing to their unique optical, electrical, and mechanical properties, but come with issues like photo corrosion and poor charge separation. Bilayer vdW heterojunctions of suitable constitutive monolayers are coming up as a potential solution to these hazards, accredited to their tunable band gap and efficient charge separation. In this paper, we have investigated the possibility of Ti_2CO_2–WX_2 (X = S, Se, Te) vdW heterostructures to perform as *Z*-scheme photocatalysts by employing first-principles density functional calculations, and thereby, the Ti_2CO_2–WSe_2 heterostructure has emerged as the most promising material for *Z*-scheme photocatalysis. Further, excited-state dynamics simulation reveals that the timescales of electron transfer and hole transfer are greater (1.13 and 1.22 ps, respectively) than the maximum time limit of the photogenerated electron–hole recombination (1.0 ps) owing to the weaker non-adiabatic coupling and electron–phonon coupling. This affirms that photogenerated electrons and holes with greater redox ability are preserved to drive the photocatalytic pathway. In addition, the free energy calculations associated with the HER and OER processes entail that the processes occur spontaneously on the surface of the heterostructure without any co-catalyst. This establishes the Ti_2CO_2–WSe_2 heterostructure as a potential mediator-free direct *Z*-scheme photocatalyst for overall water splitting.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 54
Time: Jul 5, 2023 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/92203074064?pwd=eGlCeUttNXA1dCtjc25NOEVpUVNBQT09

Meeting ID: 922 0307 4064
Passcode: 566431