VISTA Seminar

Seminar 34

March 30, 2022

10:00 am – 11:30 am EDT / 2:00 – 3:30 pm GMT /3:00 – 4:30 BST / 4:00 pm – 5:30 pm Paris

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Model Construction and TD-DMRG Simulation for Exciton Dynamics in Molecular Aggregated Systems

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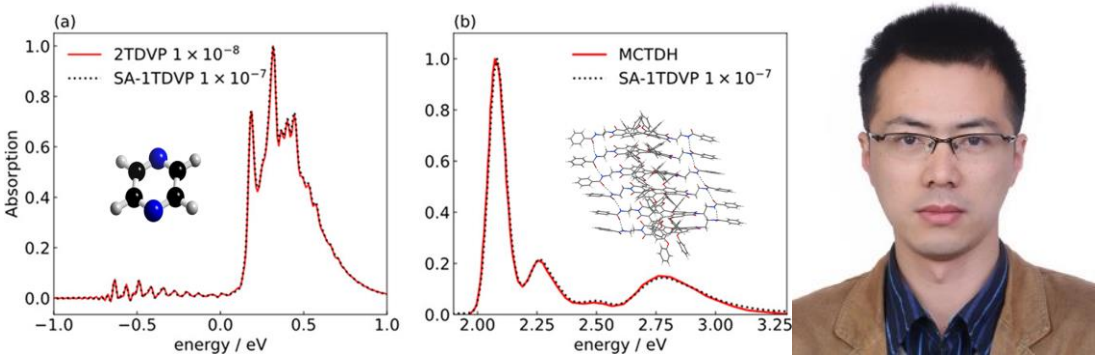

Excitonic model Hamiltonians are widely used in the theoretical simulation of excited state dynamics and spectroscopy in large photoactive systems, such as molecular aggregates in organic optoelectronic materials and biological light-harvesting systems. However, the choices of model basis and parameter values are heavily dependent on experimental fitting or empirical setting, hindering their routine applications to new chemical systems. Moreover, their real-time quantum dynamics simulations are also highly challenging for excitonic systems with strong exciton−vibration/phonon couplings due to the exponentially growing computational costs with the increasing system size. In this talk, I will introduce our recent developments of an automatic scheme for the accurate construction of the bases for excitonic models,[1] and an approximate approach for the efficient evaluation of exciton-phonon couplings.[2] I will also introduce our recent efforts on applying time-dependent density matrix renormalization group (TD-DMRG) method for real-time quantum dynamics simulations of realistic excitonic systems[3,4] with a large number of vibrational degrees of freedom, and the development of a new stochastic adaptive single-site TD-DMRG algorithm,[5] which integrates the traditional advantages of both the high efficiency of the single-site variant and the high accuracy of the two-site variant.

References

1. K. Wang, Z. Xie, Z. Luo, H. Ma, *J. Phys. Chem. Lett.* **2022**, 13, 462.
2. X. Xie, A. Santana-Bonilla, W. Fang, C. Liu, A. Troisi, H. Ma, *J. Chem. Theory Comput.* **2019**, 15, 3721.
3. Y. Yao, K. Sun, Z. Luo, H. Ma, *J. Phys. Chem. Lett.* **2018**, 9, 413.
4. X. Xie, Y. Liu, Y. Yao, U. Schollwöck, C. Liu, H. Ma, *J. Chem. Phys.* **2019**, 151, 224101.
5. Y. Xu, Z. Xie, X. Xie, U. Schollwöck, H. Ma, *JACS Au* **2022**, 2, 335.

Optical and vibrational spectroscopy of (chiral) systems with RT-TDDFT: Gauge dependence and linear response

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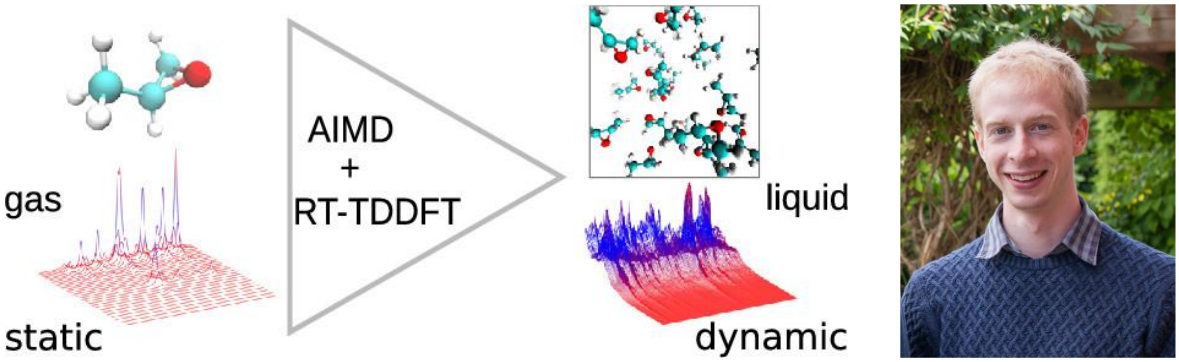

Real-time time-dependent density functional theory (RT-TDDFT) has become a widely used tool for the simulation of optical (linear) response. Apart from its favorable scaling and its capacity to resolve the entire energy domain linear response functions in one go, RT-TDDFT provides a unique framework to address the gauge dependence of practical calculations.

In this contribution recent results for UV-VIS absorption[1], electric circular dichroism[2], Raman[1] and Raman optical activity[3] are presented in unified linear response formalism, including approaches to Raman spectroscopy for the gas and liquid phase[4]. Specifically the reference point and gauge origin dependence of magnetic and quadrupolar response as well as the inherent gauge dependence stemming from the use of finite basis sets and non-local potentials are discussed.

References

[1] J. Mattiat, S. Luber, J. Chem. Phys., 149, 174108, (2018)
[2] J. Mattiat, S. Luber, Chem. Phys, 527, 110464, (2019)
[3] J. Mattiat, S. Luber, J. Chem. Phys., 151, 234110, (2019)
[4] J. Mattiat, S. Luber, J. Chem. Theory Comput., 17, 1, 344–356, (2021)

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 34
Time: Mar 30, 2022 10:00 AM Eastern Time (US and Canada)

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