VISTA Seminar

Seminar 45

November 16, 2022

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:

How the change of the ligand from porphine, P^{2-}, to P_4-substituted porphine, $P(P)_4^{2-}$, affects the electronic properties and the metal-ligand binding energies for the first-row transition metals: comparative study

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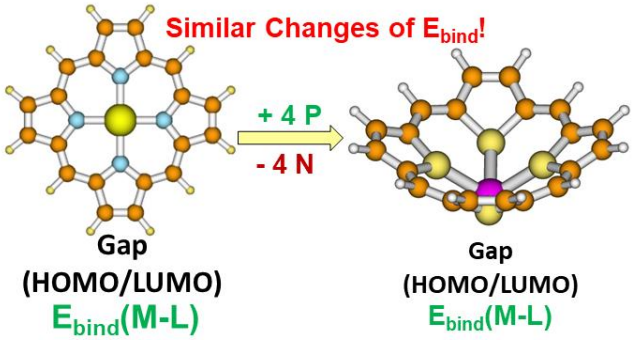

We performed comparative DFT study, including Natural Bond Orbitals (NBO) analysis, of the binding energies between all the first-row transition metals M^{n+} (M = Sc–Zn) and two ligands of the similar type: porphine, P^{2-}, and its completely P-substituted counterpart, $P(P)_4^{2-}$. The main findings are as follows: (i) complete substitution of all the pyrrole nitrogens with P-atoms does not affect the ground spin state of metalloporphyrins; (ii) generally, for the $MP(P)_4$ compounds the calculated HOMO/LUMO gaps and optical gaps are smaller than for their MP counterparts; (iii) the trends in the change of the binding energies between M^{n+} and $P(P)_4^{2-}/P^{2-}$ are very similar for both ligands. The complete substitution of the pyrrole nitrogens by the P-atoms decreases the M^{n+}-ligand binding energies; all the $MP(P)_4$ compounds studied are stable according to the calculated Ebind values and therefore can be potentially synthesized.

References

How the change of the ligand from L = porphine, P^{2-}, to L = P_4-substituted porphine, $P(P)_4^{2-}$, affects the electronic properties and the M–L binding energies for the first-row transition metals M = Sc–Zn: Comparative study. Aleksey E. Kuznetsov. Chemical Physics, 2016, 469–470, 38-48.

Molecular quantum dynamics with tensor train

Ningyi Lyu

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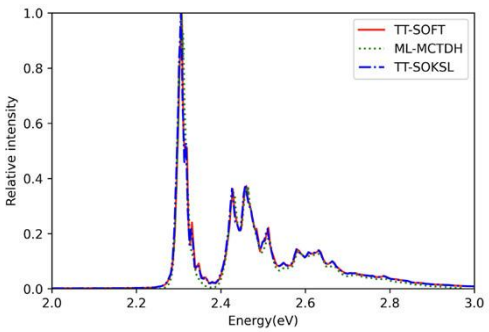

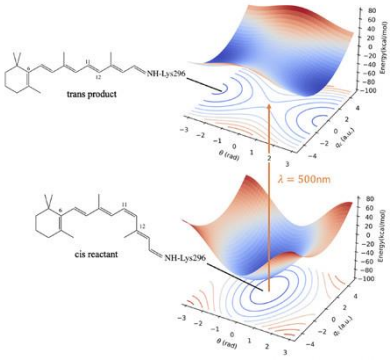

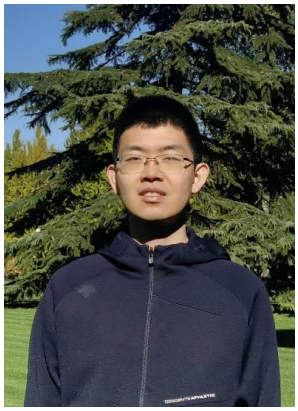

Explicitly solving the time-dependent Schrodinger equation for complicated molecular systems poses significant challenges due to the high computational cost that grows exponentially with the number of Degrees of Freedom (DoF). These challenges are tackled by tensor train methods, which numerically accurately represents the high-dimensional wavepacket as a product of 3-dimensional arrays, thereby bypassing the exponential wall. In this study, we developed a new tensor-train-based propagation method that facilitates the dynamical simulation of non-harmonic, non-adiabatic, high-dimensional molecular models. This so-called tensor-train split-operator KSL (TT-SOKSL) method successfully simulates the dynamics of a 25-dimensional 2-level model that describes photoinduced cis-trans isomerization of retinal, a reaction identified as the first step of dim-light vision. We also applied the numerically exact results produced by tensor train methods as benchmarks for both reduced methods like generalized quantum master equations (GQMEs) and approximate methods such as linearized semiclassical (LSC) methods.

References

J. Chem. Theory Comput. 18: 3327-3346 (2022) Tensor-Train Split Operator KSL (TT-SOKSL) Method for Quantum Dynamics Simulations, by Ningyi Lyu, Micheline B. Soley, and Victor S. Batista

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 45
Time: Nov 16, 2022 10:00 PM Eastern Time (US and Canada)

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