VISTA Seminar

Seminar 106

April 8, 2026

10:00 am – 11:30 am EDT Buffalo / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

Strong Correlations and Topological Transitions in Chemical Reactions

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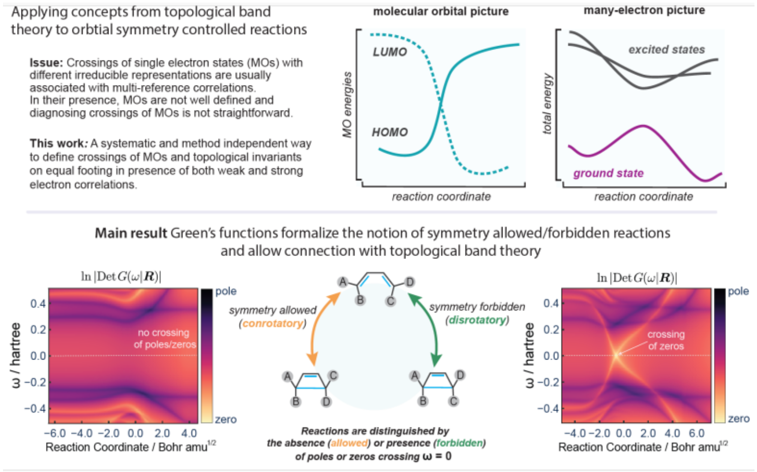

Applying concepts from topological band theory to orbtial symmetry controlled reactions

Issue: Crossings of single electron states (MOs) with different irreducible representations are usually associated with multi-reference correlations.
In their presence, MOs are not well defined and diagnosing crossings of MOs is not straightforward.

This work: A systematic and method independent way to define crossings of MOs and topological invariants on equal footing in presence of both weak and strong electron correlations.

Main result Green's functions formalize the notion of symmetry allowed/forbidden reactions and allow connection with topological band theory

Reactions are distinguished by the absence (allowed) or presence (forbidden) of poles or zeros crossing ω = 0

Classifying energy level connectivity via topological invariants has become a standard tool in condensed-matter physics. Despite many fundamental questions, extending these concepts to molecular systems has recently attracted significant interest. Reactions governed by orbital symmetry conservation are ideal candidates to test this extension, as they classify pathways as symmetry-allowed or symmetry-forbidden depending on whether molecular orbitals cross along the reaction coordinate. However, the presence of strong electronic correlations in these reactions invalidate the framework underlying topological band theory, preventing direct generalization. Here, we introduce a formalism in terms of Green's functions to classify orbital symmetry controlled reactions even in the presence of strong electronic correlations. Focusing on prototypical 4pi electrocyclizations, we show that symmetry-forbidden pathways are characterized by crossings of Green's function zeros, in stark contrast to the crossings of poles as predicted by molecular-orbital theory. We introduce symmetry-resolved invariants that provide endpoint diagnostics for symmetry-preserving paths and motivate direct zero-tracking when symmetry is weakly broken. The result is a many-body generalization of orbital-crossing selection rules and a bridge to established concepts from topological and strong interaction physics in a molecular setting.

Theory of Photoinduced Excited State Proton Transfer

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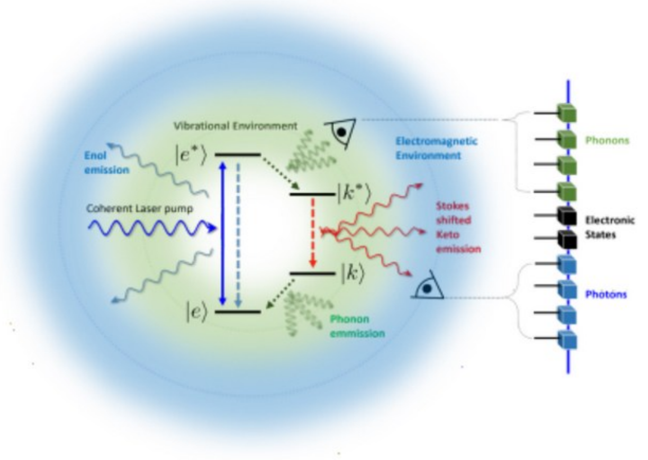

Photoinduced Excited State Proton Transfer (ESPT) is characterized by a transfer of a proton between two moieties of a molecule when the system is photoexcited, often seen via an exceptionally large Stokes shift (≥ 100 nm) in fluorescence spectra. This ultrafast process, occurring at the limit of many experimental probe timescales, plays fundamental roles in diverse biological mechanisms and provides an excellent platform for developing tailored drug delivery systems and optical devices [1]. Despite its apparent simplicity, ESPT presents significant computational challenges due to the quantum nature of nuclear motion, which cannot be neglected because of out-of-equilibrium effects occurring in the ultrafast regime. By developing simple prototype systems, we focused especially on short time behaviors parametrized by the photoexcitation shape and vibrations of the system. This surrounding environment is included with great accuracy through fully quantized theoretical simulation and powerful numerical Tensor-Network techniques [2,3], permitting us to include hundreds of vibrations modes. Studying the wavepacket propagation of test bed molecule models for ultrafast ESPT with explicit description of vibrations, we revealed the importance of the pump duration on initial conditions and on the subsequent dynamics [4]. The presented study helps gain insight into the non-equilibrium dynamics of proton transfer and provides new design principles mimicking this natural and essential process.

References

[1] P. Goyal and S. Hammes-Schiffer ACS Energy Lett. 2, 512–519 (2017).
[2] A. J. Dunnett, D. Gowland, C. M. Isborn, et al. J. Chem. Phys 155, 144112 (2021).
[3] B. Le Dé, S. Huppert, R. Spezia and A.W. Chin: J. Chem. Theory Comput. 20, 8749−8766 (2024)
[4] B. Le Dé, S. Huppert, R. Spezia and A.W. Chin: J. Phys. Chem. Lett. 16, 2514−2521 (2025)

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 106
Time: Apr 8, 2026 10:00 AM Eastern Time (US and Canada)
Join Zoom Meeting
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Meeting ID: 956 5865 7597
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nonadiabatic and quantum dynamics, as well as the applications of these cutting-edge techniques to a variety of complex systems and materials, such as solar energy harvesting and photorespons
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