

VISTA Seminar

Seminar 5

9:30 – 11:00 am EDT / 1:30 – 3:00 pm GMT

TOC:

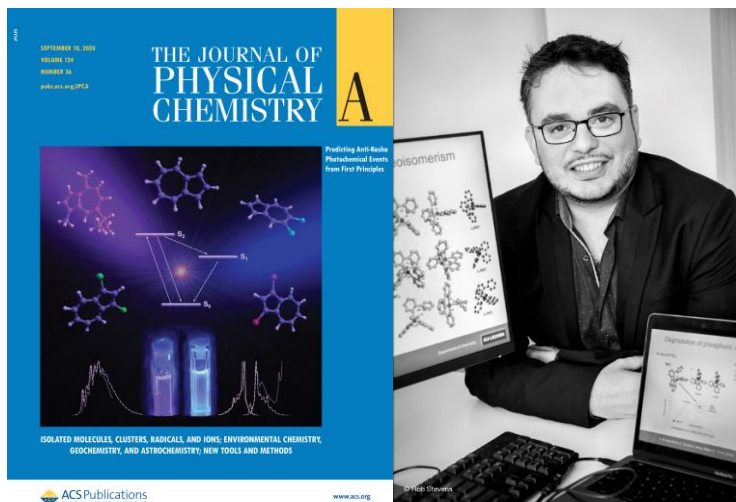
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Quantitative predictions of photochemistry from excited state decay rate calculations

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Abstract: In this contribution I present computational protocols to: predict anti-Kasha emissions in molecular systems (i.e., emissions from higher-lying excited states)[1] and to determine temperature-dependent photoluminescence lifetimes and quantum yields of phosphors.[2] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photochemistry at the first principles level.[3-4] Our protocols combine: state-of-the-art



quantum chemical calculations and excited state decay rate theories (i.e., thermal vibration correlation function formalism)[5] along with appropriate excited state kinetic models. For the anti-Kasha case, the validity of the computational protocol has been verified for a series of azulene derivatives, for which experimental data was readily available at hand. Such a protocol enables to obtain quantitative determinations of the spectra, lifetimes of the excited states and photoluminescence quantum yields of the normal and anomalous emissions.[1] For phosphors, additional photodeactivation channels including phosphorescence decay, intersystem crossing decay and non-radiative decay mediated by triplet metal-centered excited states (3MC), were considered in our kinetic model.[2] By including all relevant competing photodeactivation channels, quantitative determinations of quantum yields for Ir(III) complexes could be attained. The latter protocol is beneficial for the *in silico* pre-screening of promising OLED emissive materials.

References:

- [1] K. Veys, D. Escudero, *J. Phys. Chem. A*, 124, 7228 (2020)
- [2] X. Zhang, Q. Peng, D. Jacquemin, Z. Shuai, D. Escudero, *J. Phys. Chem. C*, 122, 6340 (2018).
- [3] M. Röhrs, D. Escudero, *J. Phys. Chem. Lett.*, 10, 5798 (2019).
- [4] D. Escudero, *Photodeactivation Channels of Transition Metal Complexes: A Computational Chemistry Perspective*. Springer International Publishing Switzerland 2019. E. Broclawik et al. (eds.), *Transition Metals in Coordination Environments. Computational Chemistry and Catalysis View points*, DOI: 10.1007/978-3-030-11714-6_9 (2019)
- [5] Z. Shuai, Q. Peng, *Phys. Rep.*, 537, 123 (2014).

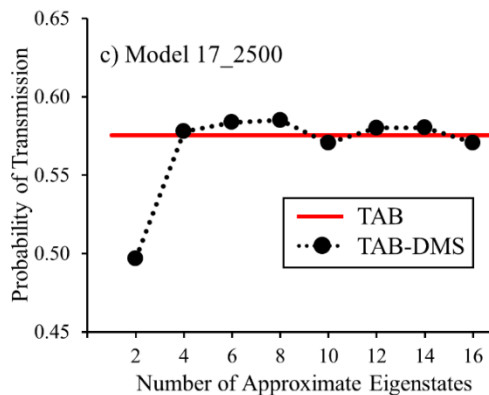
Modeling Nonadiabatic Dynamics on Many Electronic States

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Abstract: Decoherence corrections increase the accuracy of mixed quantum–classical nonadiabatic molecular dynamics methods, but they typically require explicit knowledge of the potential energy surfaces of all occupied electronic states. This requirement renders them impractical for applications in which large numbers of electronic states are occupied. Recently, we have introduced the collapse to a block (TAB) decoherence correction [1], which incorporates a state-pairwise definition of decoherence time to accurately describe dynamics on more than two electronic states. In this talk, we describe an extension to TAB, where a scheme for efficiently computing a small number of approximate eigenstates of the electronic Hamiltonian is used, eliminating the need for explicit knowledge of a large number of potential energy surfaces [2, 3]. This adaptation of TAB for dense manifolds of states (TAB-DMS) is systematically improvable by increasing the number of computed approximate eigenstates. Application to a series of one-dimensional model problems demonstrates that TAB-DMS can be consistent with TAB simulations, which employ the complete set of adiabatic electronic states, when even a very modest number of approximate eigenstates are computed. Additionally, comparison of TAB and TAB-DMS simulations to exact quantum dynamical simulations indicates that both methods are quite accurate so long as the decoherence correction is carefully parameterized.

References:

1. M. P. Esch and B. G. Levine, *J. Chem. Phys.* **152**, 234105 (2020)
2. M. P. Esch and B. G. Levine, *J. Chem. Phys.* **153**, 114104 (2020)
3. D. A. Fedorov and B. G. Levine, *J. Phys. Chem. Lett.* **10**, 4542 (2019)

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 5

Time: Nov 5, 2020 09:30 AM Eastern Time (US and Canada)

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