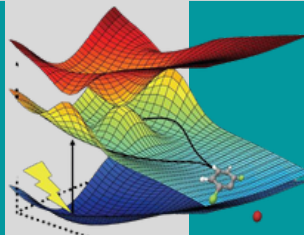


# “CHARACTERIZATION OF EXCITED STATES AND NONADIABATIC PHOTODYNAMICS FOR PARADIGMATIC POLYCYCLIC AROMATIC HYDROCARBON SYSTEMS”



## Prof. Dr. Hans Lischka

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**November 26, 2021 (Friday)**  
**12pm (BRT time) - Google Meet**

### ORGANIZATION:

#### Prof. Dr. Antonio Carlos Borin

Instituto de Química, Universidade de São Paulo (USP), SP, Brazil

### INFORMATION AND REGISTRATION:

ancborin@iq.usp.br

**Registration:** send a message to ancborin@iq.usp.br

with the words “Hans Lischka – Virtual” on the “subject”

**Deadline:** November 25, 2021 (Thursday), 06pm (BRT time)

## ABSTRACT

Hans Lischka

Texas Tech University, Lubbock, Texas, USA

The talk starts with an introductory discussion of the calculation of the nonadiabatic interaction of energy surfaces and the practical possibilities and limitations for the calculation of excited states for larger aromatic compounds. Among the many choices of computational methods, multireference configuration interaction (MRCI), density functional theory (DFT)/MRCI, the second-order algebraic diagrammatic construction (ADC(2)), time-dependent (TD) DFT and TD tight-binding DFT (TD-DFTB) are considered. Acenes, pyrene and their stacking processes to form excimers and charge transfer (CT) states will be discussed. DFT/MRCI is used to create benchmark data for the excited states of pyrene and circular extended pyrenes in comparison to ADC(2) and TD-DFT/B3LYP and CAM-B3LYP calculations. ADC(2) computes correctly the S1 state as a dark state whereas the DFT methods give a bright state as the lowest one. Excimer formation in several circum extended pyrene and coronene dimers is shown to be responsible for the large Stokes shift in carbon dots. Surface hopping dynamics calculations using ADC(2) are reported to investigate excimer formation in the benzene dimer and to study the CT dynamics in the anthracene/tetracyanoethylene complex. Pathways to Fluorescence via Restriction of Intramolecular Motion (RIM) in Substituted Tetraphenylethylenes are explored by means of TD-DFTB surface hopping dynamics.

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