

CRC 1249 – Colloquium

08.07.2026

16:15 Uhr, Hörsaal West

Prof. David Casanova

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Connecting Electronic Structure to Photophysics, Spin-state Preparation, and Energy Transfer in Molecular Systems

In this talk, I will present recent developments from our group in the electronic structure theory of open-shell molecular systems, with an emphasis on spin-dependent properties, excited states, and strong electron correlation. Specifically, I will discuss three recent contributions. First, I will present a computational protocol for the assessment of electronic couplings crucial to triplet-triplet annihilation upconversion (TTA-UC) in molecular materials and its application to the study of crystal rubrene [1]. Second, I will introduce a state-interaction framework that combines TDDFT and spin-orbit coupling to compute and interpret molecular g-matrices, providing an efficient route to describe magnetic anisotropy and spin-mixing effects [2]. Finally, I will address the optical addressability of nitrenes, highlighting the electronic-structure factors that govern spin-selective optical transitions and enable the optical initialization and readout of molecular triplet states [3]. Throughout the talk, these methodological developments will be illustrated through representative molecular case studies.

References

- [1] Diaz-Andres A., Tonnelé C., Casanova D., *J. Chem. Theory Comput.* **20**, 4288-4297 (2024)
- [2] Cebreiro-Gallardo A., Casanova D., *J. Chem. Theory Comput.* **21**, 6528-6544 (2025)
- [3] Ricci G., Tonnelé C., Casanova D., *J. Phys. Chem. Lett.* **16**, 5659-5665 (2025)

Pretalk:

Christoph Popko

(TP C14 Amirjalayer)

Computational Insights into *N*-Hetero(poly)cycles at
Metal Interfaces