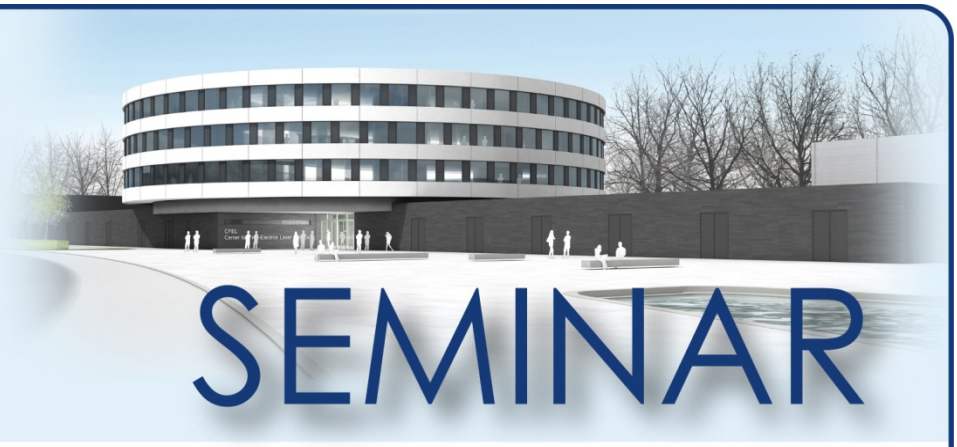
CFEL SCIENCE



SEMINAR

30 May 2024, 10:00–11:00h
CFEL (Bldg. 99) seminar room I+II

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Dealing with Multiple Electronic States: Spectroscopy, Reactivity, and Path Integral Monte Carlo

The presence of multiple electronic states with a possible multiconfigurational character plays an important role in reactivity and spectroscopy, affecting also molecular properties at finite temperatures. Such effects are particularly prominent in transition metals, being thus of interest, inter alia, for catalysis. In my contribution, I will present our recent efforts in modeling of multi-state reactivity in CO_2 activation on Ta^+, employing full-dimensional, machine-learned potential energy surface [1], with simulations verified against velocity map imaging experiments [2]. Further, I will show that the multiconfigurational character of electronic states might be, under favorable circumstances, revealed spectroscopically [3]. Finally, I will discuss how symmetry breaking might be used to reveal the electronic structure of the FeH^+ ion and argue that path integral Monte Carlo approach might be often needed to describe correctly the properties of transition metal complexes.

1. Y. Liu, M. Ončák, J. Meyer, S. G. Ard, N. S. Shuman, A. A. Viggiano, H. Guo, *J. Am. Chem. Soc.*, **146**, 14182 (2024). DOI: 10.1021/jacs.4c03192
2. M. Meta, M. Huber, T. Michaelsen, A. Ayasli, M. Ončák, R. Wester, J. Meyer, *J. Phys. Chem. Lett.*, **14**, 5524 (2023). 10.1021/acs.jpclett.3c01078
3. D. Jank, M. Ončák, S. Jin, C. van der Linde, M. K. Beyer, *J. Am. Chem. Soc.*, accepted.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar