2nd live session of seminar series **Focus Materialchemie** – Wednesday, **29.03.2023** 16:00 @ **Seminarraum Lehar 01** (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – join us on **ZOOM** (ID: 983 0066 2349)

Machine learning for multiple electronic states

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Different developments of machine learning for photochemistry simulations will be presented. Here, machine learning is employed to predict excited-state properties like potential energy surfaces, forces, nonadiabatic coupling vectors, spin-orbit couplings and transition dipole moments [1,2,3]. With these properties at hand, excited-state dynamics simulations are accelerated approximately by a factor of 1000, putting nanosecond time scales into reach. Furthermore, the combination of machine learning (ML) and molecular mechanics (MM) in an ML/MM approach for multiple electronic states will be discussed.

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1. J. Westermayr, M. Gastegger, M. Menger, S. Mai, L. González, P. Marquetand, Machine learning enables long time scale molecular photodynamics simulations, Chem. Sci., 10, 8100-8107 (2019).
2. J. Westermayr, M. Gastegger, P. Marquetand, Combining SchNet and SHARC: The SchNarc machine learning approach for excited-state dynamics, J. Phys. Chem. Lett., 11, 3828-3834 (2020).
3. J. Westermayr, P. Marquetand, Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space, J. Chem. Phys., 153, 154112 (2020).