Webinars on Computational Photochemistry

"Nonadiabatic Machine Learning Molecular Dynamics"

Priv.-Doz. Dr. Philipp Marquetand

Institute of Theoretical Chemistry,
University of Vienna, Vienna, Austria

December 04, 2020 (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 "Philipp Marquetand – Virtual" on the "subject"
Deadline: December 02, 2020 (Wednesday), 06pm (BRT time).

Universidade de São Paulo
Instituto de Química

Webinars on
Computacional Photochemistry
Prof. Dr. Antonio Carlos Borin

Nonadiabatic Machine Learning Molecular Dynamics

Philipp Marquetand

Institute of Theoretical Chemistry, Faculty of Chemistry, University of Vienna,Währinger Str. 17, 1090 Vienna, Austria
Research platform on Accelerating Photoreaction Discovery, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria
Data Science @ Uni Vienna, University of Vienna, Währinger Str. 29, 1090 Vienna, Austria

The development and application of machine learning potentials for excited states [1-3] will be presented, aiming at fast and accurate nonadiabatic molecular dynamics simulations. The dynamics is simulated with our surface hopping approach SHARC (surface hopping including arbitrary couplings), which is able to treat not only kinetic dynamical couplings but also any other arbitrary coupling on an equal footing [4]. Consequently, machine learning is employed not only for potentials and forces but also for nonadiabatic couplings, spin-orbit couplings [5-7] and dipole moments [8]. These developments open up the possibility to simulate time scales in the nanosecond regime compared to a few picoseconds in conventional approaches [5].

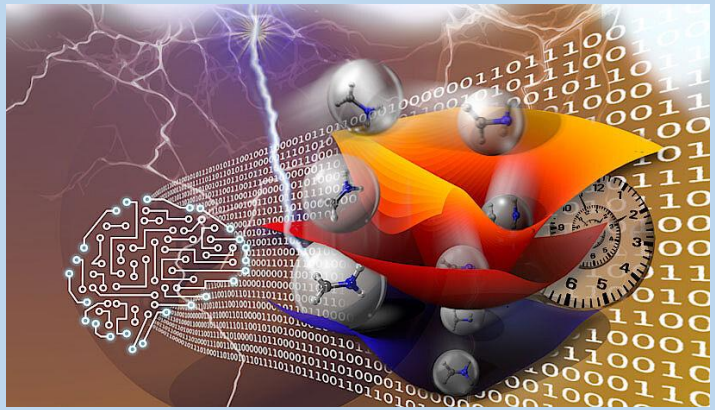

Figure 1: Machine learning enables long time scale molecular photodynamics simulations (Cover illustration, DOI:10.1039/C9SC90196E)

1. J. Westermayr, P. Marquetand, Machine Learning for Electronically Excited States of Molecules, *Chem. Rev.*, DOI:10.1021/acs.chemrev.0c00749 (2020).
2. J. Westermayr, P. Marquetand, Perspective: Machine learning and excited-state molecular dynamics, *Mach. Learn.: Sci. Technol.*, **1**, 043001 (2020).
3. J. Westermayr, P. Marquetand, Machine Learning for Nonadiabatic Molecular Dynamics, *in: Machine Learning in Chemistry: The Impact of Artificial Intelligence*, (Ed.: H. Cartwright) Royal Society of Chemistry (2020).
4. S. Mai, P. Marquetand, L. González, Nonadiabatic Dynamics: The SHARC Approach, *WIREs Comput. Mol. Sci.*, **8**, e1370 (2018).
5. 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).
6. J. Westermayr, F. A. Faber, A. S. Christensen, O. A. von Lilienfeld, P. Marquetand, Neural networks and kernel ridge regression for excited states dynamics of $CH_2NH^+_2$: From single-state to multi-state representations and multi-property machine learning models, *Mach. Learn.: Sci. Technol.*, **1**, 025009 (2020).
7. 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).
8. 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).

Universidade de São Paulo
Instituto de Química