FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

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„Artificial Neural Networks and Dynamics in Excited States"

Artificial neural networks can learn the relationship between the nuclear geometry of a molecule and the corresponding potential energy. The neural networks then serve as a highly accurate and extremely fast tool for predicting potential energy surfaces. Different applications of such neural network potentials will be shown, e.g. the computation of an organic reaction or the calculation of infrared spectra. In the future, the technique will be extended to excited states.
Currently, we still use highly accurate but time-consuming ab initio calculations to provide potentials for excited-state dynamics simulations. In the latter, we study molecules by our so-called SHARC (surface hopping including arbitrary couplings) method. The method is applied to a variety of systems, showing e.g. that intersystem crossing can take place on a femtosecond timescale even in organic molecules with only relatively small spin-orbit couplings.

Montag, 24. April 2017, 16:00 Uhr
Joseph Loschmidt Hörsaal
Währinger Straße 42, 1090 Wien

Bernhard Keppler Dekan	Lothar Brecker Vizedekan	Veronika Somoza Vizedekanin