



Einladung zum Vortrag von

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**Prof. Dr. Wolfgang Einfeld**

Universität Bielefeld

***Development of diabatic potential energy surfaces (PESs)  
for molecular quantum dynamics simulations***

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The theoretical treatment of molecular processes involving multiple electronic states requires a proper description of the potential energy as well as the couplings among the electronic states. The latter becomes particularly important whenever the dynamics is affected by conical intersections or avoided crossings. Especially the presence of conical intersections and the corresponding geometric phase effect has a significant qualitative effect on wave functions and eigenstates. One elegant way to handle such complications is the use of a diabatic representation of the electronic Hamiltonian. However, diabatic representations are not unique and thus they are not directly accessible. Therefore, several techniques and strategies have been developed how to obtain diabatic representations from standard electronic structure calculations. An overview will be presented over theoretical background and established diabatization strategies, namely wave function based vs. energy based approaches. Our recent advances in the development of diabatic PES models will be discussed, particularly our hybrid diabatization method. The power of these approaches will be demonstrated by some selected applications.

Montag, 11. März 2019, 13:30 Uhr  
Seminarraum 4. Stock  
Währinger Straße 17, 1090 Wien

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