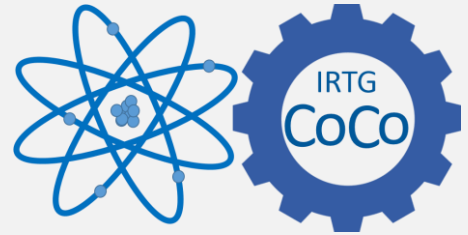


IRTG-Seminar



Dr. Ralph Gebauer

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“Optical properties of hydrogen-bonded systems: the subtle role of nuclear quantum effects”

Hydrogen bonds play an ubiquitous role in nature. While the crucial role of these weak bonds for structural and ground-state properties is universally acknowledged, much less is known about the influence of H-bonds on electronic excited states.

In this talk, I will present recent work based on ground-state molecular dynamics and excited state calculations using time-dependent density functional theory. In particular, I will focus on proton transfer processes and the role which nuclear quantum effects can play in hydrogen bonds. I will show that proton transfer across hydrogen bonds is favored by quantum effects and how such processes influence the electronic excited states. One particular example for this effect is the case of intrinsically fluorescent protein fibrils where our calculations explain the experimentally observed fluorescence even in fibrils without aromatic residues or multiple bond conjugation that characterize conventional fluorescent systems.

Ref: <http://pubs.acs.org/doi/abs/10.1021/jacs.5b11012>

**Tuesday, October 18th, 2016, 4:00 p.m., HS I,
Physics High Rise, Hermann-Herder-Str. 3**