

Physikalisches Kolloquium



Thursday, 19.10.2017, 17:15, HS 100
Reception with coffee & cookies 16:45
 (For university staff: please bring your own cup for sustainability reasons)

Dr. Igor Schapiro, The Hebrew University of Jerusalem, Israel:

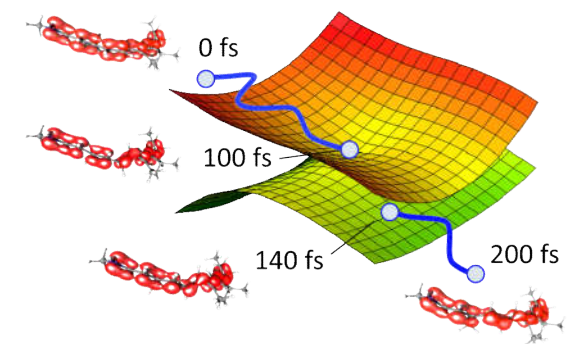
Understanding Isomerization – Insight from hybrid QM/MM molecular dynamics simulations

Abstract

The primary event of vision in the vertebrate eye is the highly selective and efficient photoisomerization of 11-cis-retinal protonated Schiff base (RPSB) bound to the visual protein rhodopsin (Rh). With a ~100% selectivity, ~65% quantum yield, and ~200 fs product appearance time, this isomerization is considered the archetype of a photochemical reaction optimized by nature to achieve a specific molecular response. Recently, we have used a combination of a quantum chemical and a classical force field method (QM/MM) to resolve the isomerization mechanism for the RPSB chromophore in Rh[1]. Important stereoelectronic factors were found that determine the outcome of the photoisomerization. The same protocol was also applied to investigate the photochemical mechanism of the newly discovered Anabaena Sensory Rhodopsin[2] and of a biomimetic molecular switch that works in solution[3]. Using the same computational protocol we have also studied the ground state (thermal) isomerization.[4] The results of the simulations explain the molecular mechanism of thermal noise in rod photoreceptors and make a direct link to experimentally found correlations for night vision.

References:

- [1] Schapiro I, Ryazantsev M N, Frutos L M, Ferré N, Lindh R, Olivucci M. J. Am. Chem. Soc. (2011), 133, 3354.
- [2] Schapiro I, Ruhman S. Biochim Biophys Acta. (2014), 1837, 589.
- [3] Léonard J, Schapiro I, Briand J, Fusi S, Paccani R R, Olivucci M, Haacke S. Chem. Eur. J. (2012), 18, 15296.
- [4] Gozem S, Schapiro I, Ferré N, Olivucci M. Science (2012), 33, 6099.



All of you interested in physics are cordially invited!

Contact: Prof. Dr. Christiane Koch, Quantum Dynamics and Control, More Information: uni-kassel.de/go/physikalisches_kolloquium