Ab initio molecular dynamic simulation of photoactive proteins in action

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Simulation of the mode of action of enzymatic proteins often requires advanced multiscale and rare event techniques. This presentation reviews two recent advancements: an adaptive multiscale approach that allows for hybrid quantum/forcefield (QM/MM) and atomistic/coarse-grain modeling with open boundaries [1, 2] and, secondly, a new path-metadynamics method to sample slow complex processes [3]. We apply these methods in combination with Car-Parrinello molecular dynamics and classical MD to study for example the photocycle of light sensitive proteins.

[1] S. O. Nielsen, R. E. Bulo, P. B. Moore, B. Ensing, *Phys. Chem. Chem. Phys.* **12**:12401 – 12412, 2010
[2] S. O. Nielsen, P. B. Moore, B. Ensing, *Phys. Rev. Lett.* **105:** 237802, 2010
[3] G. Díaz Leines and B. Ensing, *Phys. Rev. Lett.,* 109:020601, 2012.