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From fast light-activated processes in biomolecules to large-scale aggregation of membrane proteins: molecular dynamics simulations at different time and length scales

LV Schäfer*[1], M Boggio-Pasqua[2], G Groenhof[3], H Grubmüller[3], SJ Marrink[1] and MA Robb[4]

Address: [1]University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands, [2]Toulouse, France, [3]Theoretical and Computational Biophysics, Max Planck Institute for Biophysical Chemistry, Am Faßberg 11, D-37077 Göttingen, Germany and [4]Computational Photochemistry Group, Department of Chemistry, Imperial College London, UK

* Corresponding author

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Molecular dynamics (MD) simulations can yield the structural dynamics of biomolecules at a femtoseconds time resolution and, simultaneously, at atomic spatial resolution. However, due to the large computational effort involved, MD was hitherto limited to rather small systems, such as a single molecule in water, and to timescales of a few hundred nanoseconds. Furthermore, the current molecular mechanical (MM) force fields cannot describe the making and breaking of chemical bonds or light-activated processes, which requires a quantum mechanical description.

In our contribution, we will present new methodological advancements to MD, which enable to study light-activated processes in biomolecules, and the microseconds dynamics of large biomolecular assemblies. By using an ab initio mixed quantum mechanical/molecular mechanical (QM/MM) MD strategy together with explicit surface hopping between the ground state and the light-activated state, we have revealed the sequence of structural events that follow photon absorption in wild-type and mutant photoactive yellow protein (PYP), a bacterial photoreceptor. Our results show the importance of the protein environment on the photoreaction, as mutating one key amino acid in the wild type alters the photochemical reaction and leads to a different photoproduct [1].

Furthermore, by means of a new coarse-grained MD approach [3], we studied the large scale self-assembly of proteins in membranes. The new approach drastically reduces computational effort (by a factor of about 1000), yet still provides almost atomic spatial resolution. Here, we present first results for a number of membrane-anchored green fluorescent protein (GFP) molecules anchored to an explicit biological membrane.

References

1. Groenhof G, *et al.*: *J Am Chem Soc* 2004, **126:**4228.
2. Groenhof G, *et al.*: *J Am Chem Soc* 2008, **130:**3250.
3. Marrink SJ, *et al.*: *J Phys Chem B* 2007, **111:**7812.
4. Monticelli L, *et al.*: *J Chem Theory and Comput* 2008, **4:**819.