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Ab initio study of the optical properties of green fluorescent protein

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Stellingen

Belonging to the thesis

Ab initio study of the optical properties of Green Fluorescent Protein

1. Evolution and natural selection has generated a very efficient optical device and this optimization through evolution is probably a reason for the success of Green Fluorescent Protein (GFP) in biotechnology (This thesis, Chapter 1).
2. To investigate the photophysics of GFP, we employ a variety of computational methods as there is not a single theoretical approach to date, which is capable to cover the different spacial and temporal scales which characterize this complex problem (This thesis, Chapter 2).
3. The ability of optimizing the parameters of the trial wave function is crucial for the success of quantum Monte Carlo methods (This thesis, Chapter 2).
4. The protein environment and, in particular, the residues in the binding site of the chromophore can affect the spectral response of the chromophore in a dual manner. They can in principle tune the internal geometrical structure of the chromophore as well as act on the excitations more directly as some close residues may be charged or form hydrogen bond to the chromophore (This thesis, Chapter 4).
5. For all three forms of wild-type GFP, the protein environment acts to preserve an internal structure of the chromophore which is not dramatically altered with respect to the one in vacuum (This thesis, Chapter 4).
6. London dispersion forces play an important role in several chemical and biological processes: for instance they determinate the tertiary and quaternary structure of proteins and influence processes as surface adsorption (This thesis, Chapter 5).

7. Calculations of excited electronic states are nontrivial, and unfortunately there are large discrepancies between results [for the spectrum of GFP] obtained with different theoretical models.
S. B. Nielsen *et al.*, Phys. Rev. Lett. **87**, 228102 (2001).
8. Due to the advances in the computer performances and the development of efficient quantum chemical computer programs, the computation of large (> 100 atoms) molecular systems at a quantum level becomes possible.
9. Computer modelling tools must not be used as a *black box*; even if different techniques can find an agreement with a single experiment, only the results obtained with techniques having a predictive role should be considered publishable.
10. Experiments are always needed to validate the numerical results obtained; since the reality is always too complicated we need to simplify it in order to simulate it.

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