Towards effective modelling design of biomolecular probes: EPR, NMR and NLO

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In this talk I will highlight the use of multi-scale/multi-physics approaches that combine quantum mechanics (QM) with other physical principles, like wave mechanics, molecular dynamics and dielectric theory, for applications of molecular interactions and properties. Our earlier research has mostly addressed organic and organometallic compounds and semiconductor quantum particles, like quantum dots. With the combination of QM and wave mechanics we study optical control of strong laser pulses, in particular pulse propagation in non-linear media [1]. We address the optical transmission from cross sections of multi-photon absorption processes and from considerations of propagation effects, saturation and pulse effects. With the combination of QM and molecular dynamics we study nonlinear optical properties of polymeric guest-host systems [2]. The modeling involves quantum chemistry calculations to predict the properties of a single chromophore molecule and molecular dynamics simulations to model the macroscopic optical properties of the guest-host systems and to elucidate the microscopic origin behind the macroscopic properties.
In recent time we have extended this work to consider the quantum mechanics molecular dynamics response approach of Mikkelsen, Kongsted and coworkers [3] where the full QM and MM interactions are acounted for in the evaluation of a given property. The underlying structures and trajectories are obtained by molecular dynamics or Car-Parinello-MM methods. In the talk I highlight recent results on solvatochromatic effects, non-linear optical processes, EPR and NMR parameters in solution [4,5]. Some first results on protein environments are given, and a discussion on the proper MM parameterization of such environments, for effective calculations is discussed in connection to that.

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