Mixed QM/MM Car−Parrinello Simulations of Biological System

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Due to the extended size and complexity inherent to biological systems, computer simulations based on a first−principles description are a particularly challenging task. We have chosen an hierarchichal hybrid approach in which part of the system can be treated at the dynamical density functional level whereas its environment is taken explicitly into account through the coupling with an atomistic molecular mechanics representation. This type of mixed QM/MM simulations enable the investigation of chemical processes that occur in complex biological systems. In this talk, a number of case studies will be presented that illustrate the power of such a combined modelling approach.
