Interfacing CRYSTAL/AMBER to Optimize QM/MM Lennard–Jones Parameters for Water and to Study Solvation of TiO2 Nanoparticles - DTU Orbit (14/10/2019)

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Metal oxide nanoparticles (NPs) are regarded as good candidates for many technological applications, where their functional environment is often an aqueous solution. The correct description of metal oxide electronic structure is still a challenge for local and semilocal density functionals, whereas hybrid functional methods provide an improved description, and local atomic function-based codes such as CRYSTAL17 outperform plane wave codes when it comes to hybrid functional calculations. However, the computational cost of hybrids are still prohibitive for systems of real sizes, in a real environment. Therefore, we here present and critically assess the accuracy of our electrostatic embedding quantum mechanical/molecular mechanical (QM/MM) coupling between CRYSTAL17 and AMBER16, and demonstrate some of its capabilities via the case study of TiO2 NPs in water. First, we produced new Lennard–Jones (LJ) parameters that improve the accuracy of water–water interactions in the B3LYP/TIP3P coupling. We found that optimizing LJ parameters based on water tri- to deca-mer clusters provides a less overstructured QM/MM liquid water description than when fitting LJ parameters only based on the water dimer. Then, we applied our QM/MM coupling methodology to describe the interaction of a 1 nm wide multilayer of water surrounding a spherical TiO2 nanoparticle (NP). Optimizing the QM/MM water–water parameters was found to have little to no effect on the local NP properties, which provide insights into the range of influence that can be attributed to the LJ term in the QM/MM coupling. The effect of adding additional water in an MM fashion on the geometry optimized nanoparticle structure is small, but more evident effects are seen in its electronic properties. We also show that there is good transferability of existing QM/MM LJ parameters for organic molecules–water interactions to our QM/MM implementation, even though these parameters were obtained with a different QM code and QM/MM implementation, but with the same functional.

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