Large Scale QM Simulations of Periodic Systems: The Cases of Mesoporous Silica and Protein Crystals

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Recent evolutions in High Performance Computing (HPC) architectures and the concurrent development of more efficient quantum-mechanical software have dramatically increased the size and complexity of the systems that can be modeled by fully *ab initio* methods, at a very high accuracy level. One of the areas that greatly benefits from these advancements is materials science: surfaces and interfacial phenomena, defective solids, biomaterials and nano-particulate systems, all require models that are hardly handled by desktop computing architectures due to the large system size. Two recent applications of periodic large scale *ab initio* simulations will be shown: the investigation of drugs encapsulated into mesoporous silica materials for drug delivery purposes and the first fully quantum-mechanical modeling of a protein crystal, inclusive of lattice solvating water molecules.