Computational Approaches for the Modelling of Nanobiomaterials

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The exact solution of the Schrödinger equation would allow the prediction of properties at atomistic scale to an unprecedented level of accuracy. Despite the Paul Dirac's pessimistic statement that "… the exact application of these laws leads to equations much too complicated to be soluble", a great deal of work and ingenuity by theoretical chemists has transformed the "much too complicated equations to be soluble" into a manageable and efficient ensemble of algorithms to solve the Schrödinger equation. Today, the tools developed by theoretical chemists, combined with the enormous progress in computer technology, allow prediction of the physico-chemical properties for molecules within the chemical accuracy threshold (4 kJ/mol). More recently, these tools have been extended to characterize crystalline and amorphous materials as well, albeit with an inferior degree of accuracy compared to molecules. Modern high-performance computing facilities have widen the applicability of *in silico* studies to an extent that the experimental properties for crystalline materials can be supplemented with computed ones not easily amenable by direct experiments (high pressure and temperature, phase transitions, new polymorphs, etc.). Nevertheless, the application of experimental crystallographic techniques to characterize surfaces of crystalline and amorphous materials, crucial to understand phenomena like heterogeneous catalysis or soft-matter adsorption on biomaterials, is less successful than for bulk materials. In that respect, the help that computational chemist tools may provide in improving our understanding of the atomistic details occurring at the surfaces of biomaterial for their integration in living body or as drug carriers cannot be underestimated. The progress is such that we can think modern molecular modeling as a virtual microscope that allows to follow chemical process on an atomistic scale stimulating new way of thinking about complex chemical processes.