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Advanced Computational Modelling Of Interface Properties

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Extended Abstract

The current research concerns the efficient, i.e., low cost computational modelling of interface properties through the development of advanced methodologies to model interface properties in complex systems, for instance, the interaction energy between a nanomaterial and a biomolecule in a solvent. The design of materials in catalysis, energy conversion, nanomedicine and nanosafety is of great importance [1] and has significantly improved by computational materials modelling. In the present study, quantum chemical methods are used to describe electronic structure properties of material surfaces, while molecular dynamics simulations are used to compute interaction energies between the materials and chemical or biochemical compounds. The materials of interest include metals, semiconductors, carbon nanotubes, polymers, amorphous carbon and graphene. Intermolecular interactions between nanomaterials and chemical or biomolecular compounds in water are studied through molecular dynamics simulations of potentials of mean forces [2, 3], e.g., the interaction energy of a protein adsorbed on a metal surface in water is computed on the atomistic and meso-scale, where molecular and coarse grained force fields are utilised in the simulations, while water interface properties, such as the wettability of material surfaces, are obtained through molecular dynamics simulations of contact angles and immersion enthalpies [4]. Moreover, the free energy of solvation (water) including the vibrational entropy of the materials consists of a novel descriptor [5], and is examined through molecular dynamics simulations on the semi-empirical tight binding density functional theory level [6]. The interaction energies of aggregated nanoparticles in water [3, 7] and the dissolution of ions from a metal (oxide) surface are significant interface descriptors in the quest for safe materials. Latter descriptors are obtained through calculations of the free energy of the material with an atomic vacancy on the surface layer [5]. This work was funded through EU Horizon 2020 Programme, grant n^0 814572 (NanoSolveIT) and n^0 731032 (NanoCommons), and SFI grant n^0 16/IA/4506.

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