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# In Silico Characterization of Nanomaterials

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## Extended Abstract

Nanomaterials (NMs) and nanoparticles (NPs) lie at the core of many technological applications in medicine and pharmacology, as well as in the food, agriculture, electronics, and energy industries. They are also released in the environment through natural and incidental pathways. Despite our heavy reliance on NMs, the potential risk they pose to the environment and to the biological systems is still of major concern [1]. In this work, we evaluate intrinsic and extrinsic NM descriptors to aid in the prediction of biomolecular interactions at the surface of NMs and development of structure-activity relationships between their physicochemical characteristics and their toxicity [2]. Intrinsic properties are solely based on the molecular and electronic structure of the NM, while the extrinsic properties describe a NM that comes in contact with a protein in a solvent. The NM models for the calculation of intrinsic descriptors are associated with the core of the NM that is described as a periodic bulk material [2]. In this work, we present a database of calculated descriptors for several common NMs. The provided list contained various samples of NP (metals, oxides, minerals, polymers, and carbon-based compounds such as carbon nanotubes (CNTs) and graphene sheets) that were used in toxicological experiments.

The intrinsic descriptors are evaluated by different theoretical approaches. The bandgap values of all bulk NMs were calculated using density functional theory (DFT) implemented in the SIESTA package [3]. The density of states obtained from the DFT calculation at the generalized gradient approximation is used to estimate the size of the bandgap. The heat of formation, absolute hardness, electronegativity, dispersion energy, the dipole moment, the Mulliken electronegativity, the Parr and Pople absolute hardness, and polarizability descriptors were calculated using the semi-empirical PM6-D3 [4] with the MOPAC package [5]. The extrinsic (interfacial) descriptor is a quantity that describes the relative hydrophilicity/ hydrophobicity of a periodic surface NM slab (e.g. metals, metal oxides, and carbon-based NMs) in water and octanol based on the relative enthalpy of immersion. In this work, we also employ molecular dynamics with the GROMACS [6] package using e.g. CHARMM force fields [7] in order to obtain the enthalpies of the NM slab, of the solvent (water or octanol) and of the solvated slab metals, metal oxides, and carbon-based compounds. This work was funded through EU Horizon 2020 Programme, grant nº 814572 (NanoSolveIT project).

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