Hamaker Constants for Bionano Interactions in Water

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Extended Abstract

Bionano complex formation and interaction at the bionano interface are important features to understand in detail, so that a firm relationship between the nanomaterials (NMs) of any size, shape and surface charge and their biological activity in water can be established. The bulk of the NM interacts via the long-range van der Waals interaction, which is a major contribution in the calculation of the adsorption energies of biomolecules in water. Therefore, Hamaker constants are advanced descriptors of the bionano interface. We evaluate the bionano interactions through an atomistic Force Field (FF) approach. For metals we use CHARMM FF parameters [1], and for metal oxides and carbon materials as well as amino acids, lipids and sugars the FFs developed and reported [2]. All FF parameters have been applied in molecular dynamics simulations for many properties, including potentials of mean forces.

In this work, we present a methodology to estimate Hamaker constants of the bionano interface in water or just the interaction of the NM with itself in water. The long-range dispersion interaction is calculated using the Lorentz-Berthelot rules for σ and ϵ [3], i.e. combining rules that provide the interaction energy between two non-bonded atoms. By summing up all atom-atom interactions to a single parameter, the Hamaker constant between two molecular entities of the same nanoparticle (NP) can be approximated [4] by: $A_{11} = 4 \pi^2 (\rho_{NP})^2 \sum_{i \neq j} (\epsilon_{ij}(\sigma_{ij})^6)$, where ρ_{NP} is the number density of the NP, ϵ_{ij} is related to the induced dipole interactions between two particles, σ_{ij} is the effective radius between the two particles at which point repulsive interactions become important and A_{11} is the Hamaker constant for an NP interaction with itself. For A_{123}, i.e. an NP - amino acid (AA) interaction in H_2O we assume that: $A_{123} = A_{13} + A_{22} - A_{12} - A_{23}$, where A_{12}, A_{22}, A_{23} and A_{13} are the interactions of NP-AA, H_2O-H_2O, NP-H_2O and AA-H_2O respectively. All possible combinations of atom-atom interactions for the evaluation of the Hamaker constants are automatically generated with a python code requiring only the σ and ϵ parameters as well as the number density of the material.

Our rather simple approach was applied on a large number of NMs, e.g. Au, Ag and Cu, TiO_2, SiO_2, Fe_2O_3, CNTs and graphene to create a database of Hamaker constants for common nanomaterials. The calculated Hamaker constants give a very good estimate of the major interaction between the NMs and the AAs and lipid ligands consisting the building blocks of the proteins and lipids respectively. This work was funded through EU Horizon 2020 Programme, grant n° 814572 (NanoSolveIT) and n° 731032 (NanoCommons), and SFI grant n° 16/IA/4506.

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