

Multiscale Simulation of Nanofluids for Solar Thermal Energy

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Volumetric solar receivers are showing promising efficiencies as compared to traditional collectors. Many colloidal nano-suspensions (nanofluids) with enhanced optical and thermal transport properties have been investigated to directly absorb the solar radiation. However, a rational design of nanofluids for solar applications is still missing due to their multiscale nature. Here, a multiscale Coarse-Grained (CG) approach applied to nanofluids for volumetric solar receivers is introduced. By means of molecular dynamics simulations, the pair Potential of Mean Forces (pPMF) between nanoparticles is evaluated. As an exemplificative case, a couple of uncharged, alumina nanoparticles in water is considered. These results are the first steps to implement the CG force field and thus multiscale model for solar nanofluids, which may facilitate the translation of nanofluid technology from lab- to large-scale industrial production.

1 Introduction

An alternative concept for solar thermal collectors is the volumetric solar receiver, which is based on nanofluids directly absorbing the incident radiation [1]. The addition of nanoparticles to traditional fluids can drastically enhance their optical properties and improve their thermophysical performances, leading to highly efficient volumetric solar receivers. However, the multiscale nature of nanofluids makes difficult to relating nanoscale characteristics with resulting macroscopic properties. In particular, the complex mechanism of nanoparticle clustering is one of the main responsible of nanofluids stability and thus effective properties. Due to the nanoscale effects involved in nanofluids, multiscale simulation methods are needed to guide their rational design. The Coarse-Grained (CG) approach is a modelling technique able to bridge Molecular Dynamics (MD) simulations from atomistic scale to mesoscale [2]. The basic idea of coarse graining is to combine several atoms into homogeneous groups (CG beads), which interact each other by means of bonded and non-bonded interaction potentials. Here, a suitable bottom-up CG model for nanofluids is employed for directly evaluating the pPMF from MD simulations. In particular, a couple of alumina nanoparticles solvated in water is chosen as an exemplificative building block for nanofluids with solar applications.

2 Methods and Results

To evaluate the pPMF between suspended $\alpha - \text{Al}_2\text{O}_3$ nanoparticles (NPs) in water, MD simulations are carried out. The following steps describe the adopted protocol ("pulling procedure"). First, the atomistic model of each $\alpha - \text{Al}_2\text{O}_3$ NP is prepared by defining the particle geometry and atomistic force field. Specifically, 2 nm alumina spheres are hydrogenated by adding OH terminal groups on the surface. All bonds, angles and dihedral within the NP core are modeled with a harmonic potential; instead,

Lennard-Jones and Coulomb potentials are imposed for mimicking non-bonded interactions. The CLAYFF force field is adopted to distributing partial charges on the NP surface, which is neutral overall [3].

Second, two alumina nanoparticles are considered. The NPs couple is placed in a water box (22x8x8 nm) and, after energy minimization, the whole system is equilibrated at T=300 K and p=1 bar. In the first configuration, the distance between NPs center of mass (com) is set to 2 nm. Then, by restraining one particle while pulling the second one along a reaction coordinate r , a series of configurations is generated. Each configuration, which corresponds to a precise separation distance between the NPs, is taken into account for an independent 2 ns MD simulation.

Third, the pPMF is calculated by numerically integrating the interacting forces between the NPs. Results show that the minimum energy between NPs is achieved at the shortest com distance. The MD results are then compared with the DLVO theory [4]. Since we are dealing with uncharged nanoparticles, only the attractive contribution of the DLVO model is considered.

3 Conclusions

Flocculation in colloidal systems is one of the most critical aspects in the use of nanofluids for volumetric solar receivers. Here, the pair Potential of Mean Forces between two alumina nanoparticles in water is evaluated by means of MD simulations. The results show and confirm the adhesion energy between particles. The reason of such attractive interaction is mainly attributed to the London-Van der Waals forces. However, the attractive Coulomb contribution between OH groups on NPs surface should be also considered.

A complete CG model able to study nanoparticle clustering is defined by including the effects of water adsorbed at solid-liquid interface [5], nanoparticle surface charge and solution pH.

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