

PhD in Energetics

Research Title: *Modelling materials for innovative energy devices*

Funded by	DIPARTIMENTO ENERGIA
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Context of the research activity	<p>Today the efficiency of energy processes is constantly increasing due to the availability of highly efficient materials. This change is made possible mainly due to the continuous and incredible advances in nanotechnology. In particular, engineered nanoparticles are used for improving the performance of composites and colloidal suspensions, used in innovative energy devices (e.g. heat exchangers, cooling systems [1], batteries, fuel cells, etc).</p> <p>Engineered nanoparticles (<100 nm in size), their composites and their colloids, also called nanofluids, have the potential to revolutionize energy devices. Currently, many different nanoparticles are commercially available, which include 80% of the chemical elements in the periodic table. However, nanocomposites and nanocolloids are still poorly understood because of the large number of degrees of freedom and varying length/time scales involved during operation [2]. Their selection is therefore still based on a trial-and-error approach, which exploits only a small fraction of the possibilities available, by combinatorial explosion, which may include the most suitable ones. Hence the fundamental question is how nanoparticle characteristics, such as composition, size, shape, surface chemistry (including charges and coatings) and mixture composition (including compatibilizers and surfactants), determine aggregate morphology, stability, transport and surface properties</p>
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	<p>[3]. This crucial question is also a step forward for rationally assessing the toxicity and ecotoxicity of nanocomposites and nanofluids. A multiscale approach is required in order to address this challenge [4].</p> <p>References:</p> <p>[1] A review on the heat and mass transfer phenomena in nanofluid coolants with special focus on automotive applications, MB Bigdeli, M Fasano, A Cardellini, E Chiavazzo, <u>P Asinari</u>, Renewable and Sustainable Energy Reviews 60, 1615-1633.</p> <p>[2] Thermal transport phenomena in nanoparticle suspensions, A Cardellini, M Fasano, MB Bigdeli, E Chiavazzo, <u>P Asinari</u>, Journal of Physics: Condensed Matter 28 (48), 483003.</p> <p>[3] Effect of interfacial thermal resistance and nanolayer on estimates of effective thermal conductivity of nanofluids, A Khodayari, M Fasano, MB Bigdeli, S Mohammadnejad, E Chiavazzo, <u>P Asinari</u>, Case studies in thermal engineering 12, 454-461.</p> <p>[4] Multi-scale approach for modeling stability, aggregation, and network formation of nanoparticles suspended in aqueous solutions, A Cardellini, M Alberghini, AG Rajan, RP Misra, D Blankschtein, <u>P Asinari</u>, Nanoscale 11 (9), 3979-3992.</p>
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<p>Objectives</p>	<p>The objectives of the present proposal are:</p> <ol style="list-style-type: none"> 1) The PhD candidate will study the interface properties between the nanoparticles and the surrounding media (both solid and fluid), with regards to heat transfer at the nanoscale. How the Kapitza thermal resistance at the interface depends on the surface properties of the nanoparticles, on the presence of compatibilizers and surfactants and on the composition of the surrounding media will be analyzed. A multi-scale approach will be developed, including molecular dynamics, coarse-grained molecular dynamics and Brownian dynamics simulations (the latter only for fluids), to span a wider range of length and time scales and hence to provide more meaningful estimates of the thermal properties. 2) In particular, in case of nanocolloids, the PhD candidate will extend current colloidal theories (e.g. DLVO) in order to include nanoscale effects (e.g. discrete solvent effects) in modeling nanoparticles interactions and hence to produce more reliable estimates of the nanoparticles dynamics in real surrounding media. The adopted methodology will take advantage of a recently-proposed multi-scale integrated
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	<p>framework [4], based on molecular dynamics (MD), coarse-grained molecular dynamics (CGMD) and Brownian dynamics (BD) simulations.</p> <p>3) The PhD candidate will investigate molecular properties of the proposed innovative technologies for thermal storage which involve the use of nanoparticles, namely nanocomposites and nanofluids, in particular the impact of their aggregation and of the shape of the aggregates. A better theoretical knowledge of the nanoparticles aggregation allows a more effective exploitation of nanoparticles for increasing the heat transfer and the heat storage performances. Moreover also the impact on wettability properties of nanocomposite surfaces will be investigated.</p> <p>4) Finally, the PhD candidate will apply the developed theories to study optimized materials for innovative energy devices, covering a broad spectrum of applications.</p>
Skills and competencies for the development of the activity	<p>Expertise in heat and mass transfer and applied thermodynamics is mandatory. Previous experience with molecular dynamics (MD) technique and software is required, and a proved experience with LAMMPS (or GROMACS) will be a plus. Proficiency in high-level programming language (e.g. Matlab, Python) is definitively advantageous. Good understanding of the physics of nanostructures and previous experience with high-performing computing (HPC) is highly desirable.</p>