Dr. Pietro Asinari
Professor, Politecnico di Torino

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Birck Nanotechnology Center
Room 1001

Multi-scale Modelling of Nanoparticle Suspensions

Authors: Annalisa Cardellini, Matteo Alberghini, Matteo Fasano, Eliodoro Chiavazzo, Pietro Asinari

Self-assembly of nanoparticles (NPs) into mesoscopic ordered structures plays a crucial role in a large variety of applications including pharmaceutical, food, drug delivery, immunology and technological. On the one hand, trying to prevent and avoid the self-organization of nanoparticles has traditionally been the main issue for stabilizing nano-suspensions, foams and emulsions. On the other hand, the aggregation of building-blocks into mesoscopic structures has allowed to explore new materials with desired functionalities and properties. For example, many experiments and some theoretical studies have shown that the chain-forming morphologies in nano-suspensions allow an enhancement of thermal properties [1]. However, due to the challenges of controlling the multiscale phenomena occurring in nano-suspensions, clear guidelines for their rational design are still missing. Despite a wide range of experimental observations, there is an increasing need to establish rigorous modelling techniques, able to explore and describe the multiscale nature of nano-suspensions [2].

In the present work a multiscale modelling approach is implemented to relate the nanoscale phenomena to the macroscopic bulk properties of nano-suspensions. Specifically, Molecular Dynamics (MD) simulations and Brownian Dynamics (BD) are synergistically integrated to understand the mechanisms driving the building-block interactions and hence to predict the shapes of assembled clusters. First, the pair Potential of Mean Forces (pPMF) is computed between atomistic modelled NPs dispersed in aqueous solutions. A sensitivity analysis is carried out by altering the hydrophilicity of the nanoparticles, their surface charge and the salt concentration of the bulk solutions. The role of anionic (Sodium Dodecyl Sulfate -SDS-) and cationic (Dodecyl Trimethyl Ammomium -DTAB-) surfactants is also investigated. Second, Brownian Dynamics simulations are carried out to understand how nanoscale phenomena, like the hydration layer or steric interactions, affect the mesoscale dynamics.

The Coarse Grained procedure here suggested offers a practical multiscale approach for guiding a robust and optimal design of nanoparticle suspensions.

Pietro Asinari's short bio: Pietro Asinari received his B.S. and M.S. (summa cum laude) in Mechanical Engineering in 2001 and his Ph.D. in Energetics in 2005 from Politecnico di Torino. In 2005, he won the ENI Award. He is the Director of the Multi-Scale Modeling Laboratory - SMaLL - (www.polito.it/small) and Full Professor of Heat and Mass Transfer. He is member of the operational management board of the European Materials Modelling Council - EMMC - (http://emmc.info) and operational team manager of the working group on discrete modelling of materials. He is member of the International Scientific Committee of the International Conference for Mesoscopic Methods in Engineering and Science (ICMMES, https://www.icmmes.org) and member of the Editorial Board of the international journal Heliyon (http://www.heliyon.com/). He is the Principal Investigator of many national projects about materials modelling (including THERMALSKIN and NANOBRIDGE) and Unit Leader of many European projects (including EMMC-CSA, MODCOMP and COMPOSELECTOR). His research interests include heat and mass transfer; transport theory; kinetic modelling; classical molecular dynamics; extended thermodynamics; numerical modelling & HPC. Since 2002, he has (co-) authored over 90 publications about multi-scale modelling in nanotechnology and biotechnology (citations: 1572 and h-index: 25, according to Google Scholar).