MSc Thesis Project

Molecular Dynamics Simulations of Nanoparticles Stabilization

The stabilization of nanoparticles in aqueous suspensions is required in many manufacturing processes such as pharmaceutical products formulation and food engineering. A typical approach to stabilize nanoparticles is the addition of stabilizers that will form sufficiently strong barriers to prevent agglomeration (See Figure 1.a). However, stabilizers selection is still based on empirical, expensive and time consuming experimental approaches, and the mechanisms behind nanoparticle stabilization are poorly understood. To tackle these issues, molecular dynamics will be used to model nanoparticle-stabilizer interactions and to quantitatively predict the performance of the stabilizers.

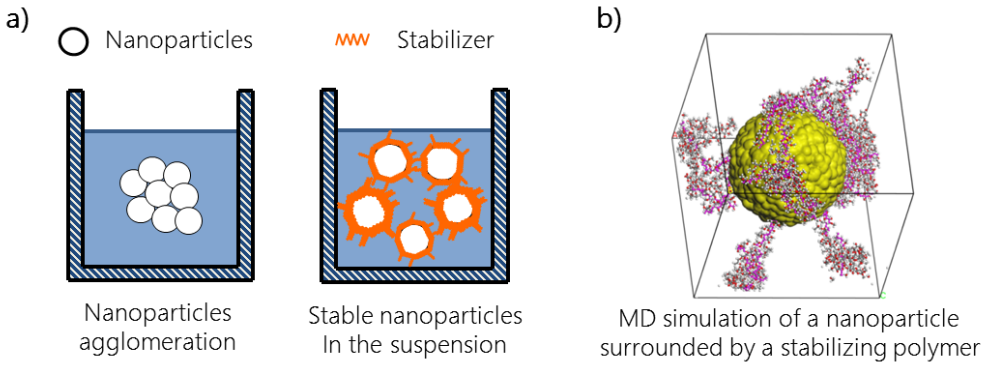

Figure 1. a) Schematic representation of the stabilization of nanoparticles, b) MD simulation of a silica particle surrounded by HPMC polymer.

Main Goal: Understand nanoparticles stabilization mechanism at the atomic-scale and select the most adequate stabilizers for industrially relevant nanoparticles.

Method: The stabilization mechanism and efficiency of nanoparticles in aqueous suspensions will be explored through two interconnected molecular dynamics approaches. The first approach is based on the computation of the Hansen solubility parameters. This will reveal the affinity between the stabilizers and the nanoparticles in the suspension and allow the selection of the most promising stabilizers. Once adequate candidate stabilizers are selected, the mechanisms of nanoparticles stabilization will be explored. Several parameters will be varied, e.g. nanoparticle size, stabilizer concentration and type, and particle surface properties, with the goal to gain an in-depth understanding of the underlying processes on the nanoscale, that is the mechanisms of stabilizer association to the nanoparticle, the interplay between the solvent and the stabilizers, and the distribution of stabilizers molecules near the nanoparticle.

Relevance: Besides its intrinsic scientific interest, a sound understanding of the mechanism of nanoparticle stabilization at the molecular scale may accelerate pharmaceutical drug development and delivery, and allow the design of new stabilizers tailored for a specific type of nanoparticles.

Collaboration: The project is a collaboration between the University of Twente (Enschede, Netherlands) and the iPAT Institute (Braunschweig, Germany). Visits to both facilities may be scheduled during the project.

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