Kinetic simulations of nanoparticle precipitation: an application to cement hydration

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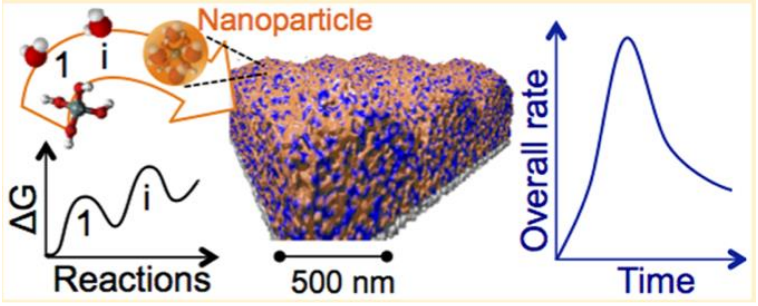
The current models of cement hydration are mostly focused on microstructure development at scales above the micrometre. There is however technological interest in controlling the texture and properties of cement hydrates below the micrometre level: at the nanoscale. The length-scales and timescales involved in cement hydration however challenge all typical simulation techniques at the nanoscale, e.g. molecular dynamics. This presentation will explore opportunities from coarsegrained simulations. Spatial coarse-graining leads to model structures that capture some complex experimental features, such as nanopore distribution, correlations from scattering experiments, and mechanical indentation moduli. Temporal coarse-graining then is proposed in the framework of Transition State Theory and Kinetic Monte Carlo, where both the chemical environment and the mechanical interactions determine the mesostructural evolution of the material. First results on predicted hydration rate of cement hydrates will be discussed, as well as implications for other mesostructured engineering materials such as zeolites and rubber-based tyre compounds.



Schematic of the new Kinetic Monte Carlo algorithm and resulting rate curve