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Kinetic Monte Carlo simulations of nanoparticle island growth[1]
BRADLEY HUBARTT, JACQUES AMAR, University of Toledo — In recent studies of the self-assembly of dodecanethiol-coated Au nanoparticle (NP) islands dissolved in toluene, the island-size distribution (ISD) was found to be quite sharp - despite the fact that island diffusion and coalescence are expected to lead to a broad ISD - while the island density was found to be anomalously low. In order to understand this, we have first used molecular dynamics (MD) simulations of a simplified model of islands adsorbed at an interface in order to study the dependence of the island diffusion coefficient on island-size. In order to understand island stability, we have also carried out additional MD simulations using an effective potential which takes into account the van der Waals and ligand-ligand interactions, which indicate that the rate of dimer break-up is surprisingly large. By including these results in kinetic Monte Carlo simulations we have obtained reasonable agreement with experiment.

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