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Self-assembly of gold nanoparticles at water/vapor interface
GARY S. GREST, J. MATTHEW D. LANE, Sandia National Laboratories — The self-assembly of coated gold nanoparticles at the water/vapor interfaces are studied using explicit-atom molecular dynamic simulations. While it is often assumed that uniformly coating spherical nanoparticles with short organic ligands lead to symmetric nanoparticles, we find that the high curvature of small nanoparticle and the relatively short dimensions of the coatings can produce highly asymmetric coatings. At an interface this asymmetry of the ligands tends to orient the nanoparticles with the surface to minimize free energy. First esults for individual gold nanoparticles of diameter 2-8 nm coated with alkanethiol ligands of various lengths and different end group will be presented. Results for the self-assembly of the multiple nanoparticles at the water/vapor interfaces will then be presented for the diameter 2 and 4 nm nanoparticles which show how these asymmetric and oriented coatings affect the interactions between nanoparticles and the structure of the resulting aggregate. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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