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Understanding electrostatic trapping of nanoparticles HUANXIN WU, ERIK LUIJTEN, Northwestern University — In electrostatic trapping, nanoparticles are polarized by the nonuniform electric field between two nanoelectrodes. The resulting dielectrophoretic (DEP) force attracts the nanoparticles to locations where the field is maximum or minimum, depending on the nanoparticle permittivity. Coarse-grained molecular dynamics simulations are often used to study such electrokinetic effects, but face the challenge of fully resolving the polarization charges and DEP forces. We extend the iterative dielectric solver developed by Barros and Luijten [*Phys. Rev. Lett.* ***113****, 017801 (2014)*] to simultaneously compute the polarization of both equipotential surfaces and dielectric objects. We apply our new algorithm to study the electrostatic trapping of nanoparticles with polarization effects resolved dynamically throughout the simulation. This method represents a new tool for design and study of collective motion of nanoparticles in DEP self-assembly.

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