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A hybrid particle-field (HPF) simulation method for polymer-nanoparticle composites DOMINIK DUECHS, UC Santa Barbara, SCOTT SIDES, Tech-X Corp., GLENN FREDRICKSON, UC Santa Barbara — A hybrid particle-field (HPF) simulation method for composite systems of polymers and sets of movable particles is presented. The particles are implemented as cavities in an otherwise flat density profile of the polymeric background (corresponding to overall incompressibility), enabling a common treatment of both components in the general framework of well-known self-consistent field theory (SCFT). The particle movements are controlled by force-biased and, where applicable, torque-biased propagation schemes. Particles and polymers interact via local contact interactions originating at the particle surfaces. Simulations with orientationally homogeneous spheres as well as with spheres possessing two distinct sets of interaction parameters on their two hemispheres are compared to experimental results.

Dominik Duechs
UC Santa Barbara

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