Dynamic Computation of Dielectric Effects in Self-Assembly and Active Matter

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The ability of matter to self-organize in complex dynamic structures is increasingly used to generate new, active materials. Progress in this field critically depends on the predictive capabilities of reliable and efficient computer simulation strategies. We have recently developed such methodologies for the coupling of dielectric solvers with particle-based simulations, making possible dynamic simulations that fully incorporate self-consistently calculated polarization charges. I will introduce our approach and discuss how the impact of these developments ranges from the prediction and control of colloidal and nanoscale self-assembly and aggregation to the understanding of dynamical properties of self-propelled particles that form the basic building blocks of active matter.

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