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The structures and energetics of interacting ionic nanocrystals from atomistic simulations.[1] PAUL TANGNEY, Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, Molecular Foundry, Lawrence Berkeley National Laboratory and Department of Physics, University of California at Berkeley — Self-assembled ordered aggregates of nanocrystals (NCs) of many different sizes, shapes and compositions have been synthesized in recent years. These "supercrystals" form a new class of material with potentially new and useful properties in which nanoparticles take the place of atoms as the fundamental building blocks of matter. However, at present neither the detailed structures of NCs themselves nor the interactions between them are well understood and it is not yet clear which forces are responsible for binding and ordering them in supercrystals. In this work, NCs of highly ionic materials are simulated using first principles molecular dynamics (MD) and MD based on accurate polarisable force-fields. Individual NCs and multiple NCs in close proximity are simulated and their structures and the electrostatic contributions to their energetics are studied in detail. From our understanding of NCs in this ionic limit we provide insight into the importance of electrostatic contributions to NC bonding in more covalent materials.

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