Abstract Submitted
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Strain in Layered Nanocrystals YOUIR BAE, RUSSEL CAFLISCH, UCLA — Layered nanocrystals consist of a core of one material surrounded by a shell of a second material. We present computation of the atomistic strain energy density in a layered nanocrystal, using an idealized model with a simple cubic lattice and harmonic interatomic potentials. These computations show that there is a critical size r_* for the shell thickness r_s at which the energy density has a maximum. This critical size is roughly independent of the geometry and material parameters of the system. Moreover it agrees with the shell thickness at which the quantum yield has a maximum, as observed in several systems.

Russel Caflisch
UCLA

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