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Designing entropy-driven binary ordered superlattices from polyhedral nanoparticles MIHIR KHADILKAR, FERNANDO ESCOBEDO, Cornell University — While ordered multicomponent structures of nanoparticles are certainly desirable in view of multiple potential applications, their self-assembly often requires highly tuned enthalpic interactions between the different constituents. We present simulation results[1] on binary mixtures of hard polyhedral nanoparticles that form ordered superlattices without any enthalpic interaction, with the help of shape anisotropy alone. We also identify a rule that maximizes packing compatibility and hence promotes the formation of ordered superlattices based on the order-disorder transition pressures of the pure components. Results show formation of plastic solid solutions in the case of binary mixtures involving nanoparticle shapes from the truncated cube family, whose pure-components also form plastic crystals. Preliminary results for 2D systems will also be presented.

[1]Mihir R. Khadilkar, Fernando A. Escobedo, **Phys. Rev. Lett. 113**, 165504 (2014)

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