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Multiscale simulations of self-assembly of CdTe nanoparticles into sheets ZHENLI ZHANG, ZHIYONG TANG, NICHOLAS KOTOV, SHARON GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, USA — By controlling the organic stabilizers on the surfaces of CdTe nanodots, these particles are found in experiments to self-assemble into one-dimensional wires and two-dimensional sheets[1,2]. To explore the underlying mechanisms for the two processes we perform simulations on multiple scales ranging from quantum mechanics to mesoscale stochastic simulations[2,3]. The simulations and corresponding energy analysis demonstrate that a delicate balance of anisotropic forces between nanoparticles is responsible for the different nanostructures they form. In particular, we show how nanoparticle shape, directional hydrophobic attraction, and electrostatic interactions determine the anisotropy of the interaction and final self-assembled structures. [1] Tang ZY, Kotov NA, Giersig M, Science, 297, 237-240, 2002. [2] Tang ZY, Zhang ZL, Wang Y, Glotzer SC and Kotov NA, Science, 314, 274-278, 2006. [3] Zhang ZL, Tang ZY, Kotov NA and Glotzer SC, preprint.

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