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Mechanism of Asymmetric Growth of Wurtzite Nanostructures: A Case Study of CdSe Through Ab Initio Computations GHANSHYAM PILANIA, RAMAMURTHY RAMPRASAD, University of Connecticut — An interesting and potentially useful phenomenon observed in wurtzite semiconductor nanocrystals is asymmetric anisotropic growth. This property has been exploited in the preferential creation of nanorods, nanoribbons and nanosaws over spherical nanocrystals. However, the details of the mechanism underlying this phenomenon of asymmetric anisotropic growth remain poorly understood. Here, we use CdSe as a prototypical wurtzite system, and oxygen as an agent that encourages asymmetric anisotropic growth. This study focus on the impact of the ordering of the surface energies of several polar and nonpolar surface facets as a function of (i) the chemical potential of Cd (i.e., precursor concentration), (ii) the presence of oxygen adsorbates, (iii) the binding modes of oxygen at the surface, and (iv) the density of oxygen adsorbates on the surfaces, using density functional theory (DFT). Our results show that by controlling the ordering of the surface energies (e.g., though proper choices of precursor concentration, temperature, and surfactants), novel growth modes such as asymmetric growth can be made possible.

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