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Effect of Hydrogen Bonding on Colloidal Nanocrystal Growth: The Case for PbS LIXIN ZHANG, National Renewable Energy Laboratory, Golden, CO 80401, SHENGBAI ZHANG, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180 — The adsorption of methylamine (CH_3NH_2) on rocksalt PbS(111)-S surface is studied by first-principles total energy calculation. It was found that nitrogen lone pairs on the CH_3NH_2 can form dative bonds with surface sulfur atoms. Such an interaction is unique in two ways: first it is non-local. Charge transfer takes place from CH_3NH_2 not only to the closest S but also to surface S further away. Second, the interaction is strongly affected by hydrogen bonds formed between CH_3NH_2 and solution molecules such as H_2O. Only by the latter effect can the PbS nanocrystals assume the (111) facets in a colloidal growth in agreement with experiment. In the past, studies of nanostructures have taken the assumption that, in the presence of a solution, the relative stability among the various facets will not change, at least not dramatically. Our study shows that such an assumption is not necessarily true. The significance of the study therefore goes beyond just the PbS or PbTe systems. Its basic principles should apply to most colloidal growth of solid-state nanostructures with broad implications.

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