

Abstract Submitted
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Density functional Study of {210}-Faceted Pd Nanocrystals in Polyvinylpyrrolidone Solution YUSHENG HOU, Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA, WENPEI GAO, XIAOQING PAN, Department of Materials Science and Chemical Engineering, University of California, Irvine, California 92697-2700, USA, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California 92697-4575, USA — Nanostructures with well-defined sizes and shapes can potentially realize a plethora of unique applications, such as sensing, catalysis, photonics, electronics, and medicine. It is highly desired that specified shapes and sizes of nanocrystals can be engineered by utilizing structure-directing agents. Our experimental measurements showed that the metal Palladium (Pd) nanostructures have more stable {210}facets in the polyvinylpyrrolidone (PVP) solution, which is different from the Pd nanoclusters in vacuum. Based on the density functional theory (DFT) along with the van der Waals (vdW) correction, we have studied the interaction of a 2-pyrrolidone (2P) ring, a submolecule of PVP, with various Pd surfaces. Our calculations indicate that 2P binds to the Pd surface via the oxygen, more strongly to the {210}facet than to {001}and {111}facets. As a result, the {210}facet becomes the preferential orientation so the Pd nanoclusters may grow in a star-shape, which explains our experimental observations.

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