Abstract Submitted
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First-Principles Calculations of the Role of PVP in the Controlled Synthesis of Au Nanostructures[1] SHIH-HSIEN LIU, Penn State University, WISSAM AL-SAIDI, University of Pittsburgh, KRISTEN FICHTHORN, Penn State University — Structure-directing agents such as PVP play an important role in determining the shape of metal nanostructures in solution-phase syntheses. It is usually hypothesized that structure-directing molecules bind more strongly to certain crystal facets, which grow at the expense of facets on which they are less strongly bound. In this study, we use dispersion-corrected density functional theory to resolve the role of PVP in the shape-selective synthesis of Au nanostructures. We calculate binding energies for the 2-pyrrolidone ring of PVP on Au(111), (5 $\times$ 1) Au(100)-hex, and Au(100) slabs in vacuum. The results show that there is no significant difference between the binding of 2-pyrrolidone to Au(111) and Au(100)-hex, while 2-pyrrolidone binds more strongly to Au(111) than to Au(100). We discuss the origins of these trends. Our results are consistent with experiments, in which (111)-faceted Au nanostructures are formed with the assistance of PVP.

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