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Adsorption of polyvinylpyrrolidone on Ag surfaces: Insight into the workings of a structure-directing agent[1] WISSAM AL-SAIDI, University of Pittsburgh, HAIJUN FENG, KRISTEN FICHTHORN, The Pennsylvania State University — We use density-functional theory to resolve the role of polyvinylpyrrolidone (PVP) as a structure-directing agent in the shape-selective synthesis of Ag nanostructures. We identify several different binding states for PVP segments on Ag(100) and Ag(111) and find an energetic preference for Ag(100), which arises from a surface-sensitive balance between direct binding and van der Waals attraction. At the chain level, correlated segment binding leads to a strong preference for PVP bind to Ag(100). Our study underscores differences between small-molecule and polymeric structure-directing agents.

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