

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Morphological Control in the Synthesis of Silver Nanostructures:
Role of Polyvinylpyrrolidone¹** KRISTEN FICHTHORN, HAIJUN FENG, RA-
JESH SATHIYANARAYANAN, Penn State University — Solution-phase syntheses
are useful for assembling metallic nanostructures with desired morphologies. For
example, a wide variety of silver nanostructures have been synthesized in the polyol
process [1], including nanowires, nanoplates, cubes, etc. Polyvinylpyrrolidone (PVP)
plays a key role in controlling nanostructure morphologies in these fabrication pro-
cesses. Based on experimental observations, the interaction strength between PVP
chains and Ag atoms in different crystallographic facets is expected to vary signif-
icantly and this shape selectivity is expected to play a key role in directing the
formation of various nanostructures. Using first-principles calculations based on
density-functional theory including van der Waals interactions, we compute the in-
teractions of the basic elements of a repeat unit in PVP (2-pyrrolidone and ethane)
with various crystal faces of Ag. Our results indicate that PVP does exhibit the ex-
pected structure sensitivity and that this arises from an interesting balance between
van der Waals interactions and direct chemical bonding. We discuss the ramifica-
tions of our calculations for the assembly of Ag nanostructures.

[1] B. Wiley et al., Chem. Eur. J. 11, 454 (2005).

¹Supported by DOE Grant # DE-FG0207ER46414.

Kristen Fichthorn
Penn State University

Date submitted: 03 Jan 2011

Electronic form version 1.4