Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Design of Janus Nanoparticles with Atomic Precision QIANG SUN, Peking University, QIAN WANG, PURU JENA, Virginia Commonwealth University, YOSHI KAWAZOE, Tohoku University — Janus nanoparticles, characterized by their anisotropic structure and interactions have added a new dimension to nanoscience because of their potential applications in biomedicine, sensors, catalysis and assembled materials. The technological applications of these nanoparticles, however, have been limited as the current chemical, physical, and biosynthetic methods lack sufficient size and shape selectivity. We report a technique where gold clusters doped with tungsten can serve as a seed that facilitates the natural growth of anisotropic nanostructures whose size and shape can be controlled with atomic precision. Using ab initio simulated annealing and molecular dynamics calculations on Au_nW (n>12) clusters, we discovered that the $W@Au_{12}$ cage cluster forms a very stable core with the remaining Au atoms forming patchy structures on its surface. The anisotropic geometry gives rise to anisotropies in vibrational spectra, charge distributions, electronic structures, and reactivity, thus making it useful to have dual functionalities. In particular, the core-patch structure is shown to possess a hydrophilic head and a hydrophobic tail. The $W@Au_{12}$ clusters can also be used as building blocks of a nano-ring with novel properties.

Qiang Sun
Peking Univeristy

Date submitted: 05 Nov 2007 Electronic form version 1.4