Abstract Submitted
for the OSF09 Meeting of
The American Physical Society

Thermodynamic properties of gold nanoparticles described by Sutton-Chen potential and Quantum Sutton-Chen potential YONGJIN PARK, GUSTAVO CARRI, Department of Polymer Science, The University of Akron — Thermodynamic properties of gold nanoparticles (<1.6nm) have been investigated by atomistic Monte Carlo simulations with three different potential functions/parameterizations (Sutton-Chen potential, Sutton-Chen potential with Pawluk's parameterization, and Quantum Sutton-Chen potential). The melting temperature of gold nanoparticles is predicted and compared to other theoretical and experimental values. The agreement between the predicted melting temperatures and the experimental values was not satisfactory for any of the three potentials in the studied range of sizes. However, the Sutton-Chen potential showed very good agreement for nanoparticles larger than 1.3nm while the Quantum Sutton-Chen potential exhibited a trend of melting temperatures similar to the experimental one although it consistently overestimated the melting temperatures.

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Date submitted: 09 Sep 2009 Electronic form version 1.4