Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Structure and dynamics of Au/Fe nano-structures: results of molecular dynamics simulation** TIMOTHY FINDLING, AHLAM AL-RAWI, Department of Physics, University of Central Florida — Gold-plated iron nanostructures have chemical, optical, magnetic, and biomedical applications owing to the unique properties of the iron-gold combination. However, relatively little is known about the atomistic surface composition of these alloys. We have studied the structure and dynamics of Au/Fe nano-alloys using molecular dynamics simulations with an embedded-atom interaction potential [1]. We will present analyses of the structural composition as Au atoms are deposited on Fe facets, leading to locally optimal crystal structures for this alloy, as a function of composition and substrate temperature. We will also present a complete analysis of the stability of the resulting structures by calculating the vibrational density of state using velocity autocorrelation. The vibrational entropic contributions to the free energy of the Fe atoms and Au atoms in their vicinities will be evaluated as a function of the local surface geometry. The net outcome of this study is prediction of viable Au/Fe nanostructures.

[1] S. M. Foiles et al. Phys. Rev. B 33, 7983 (1986).

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Date submitted: 18 Nov 2012 Electronic form version 1.4