Curvature effect on the interaction between folded graphitic surface and silver clusters

A. F. Kemper and H-P. Cheng
Department of Physics and the Quantum Theory Project, University of Florida, Gainesville, FL 32611, USA

N. Kébaïli, S. Benrezzak, M. Schmidt, A. Masson and C. Bréchignac
Laboratoire Aimé Cotton, CNRS, Univ Paris-Sud 11, Bat 505, Campus d'Orsay, 91405 Orsay Cedex, France

Evidence of curvature effects on the interaction and binding of silver clusters on folded graphitic surfaces has been shown from both experiment and theory. Density Functional Theory (DFT) calculations within the local density and generalized gradient approximations have been performed for the structural relaxation of both Ag and Ag_2 on curved surfaces, showing a cross-over from quantum to classical behaviour. Using Lennard-Jones potential to model the interaction between a single cluster and the graphene surface, evidence is found for the curvature effect on the binding of silver nano-particles to folding graphitic surfaces. The theoretical results are compared to SEM and AFM images of samples obtained from pre-formed silver cluster deposition on carboneous substrates exhibiting anisotropic pleat structures.

PACS numbers: 31.15.es, 36.40.Sx, 61.48.De

This work was supported by DOE grants DE-FG02-02ER45995 and DE-FG02-97ER45660. We would like to thank John J. Rehr for stimulating discussions.