Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Adsorption Configurations of Carbon Monoxide on Gold Monolayer Supported by Graphene or Hexagonal Boron Nitride Film: A First-Principles Study LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182, JIAXIN ZHENG, JING LU, State Key Laboratory for Mesoscopic Physics and Department of Physics, Peking University, Beijing 100871, P. R. China, PETER DOWBEN, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, NE 68588 — Using density functional theory with a semiempirical van der Waals approach proposed by Grimme, the adsorption behavior of carbon monoxide on a gold monolayer supported by graphene or monolayer hexagonal boron nitride has been investigated. Based on the changes in the Dirac cone of graphene and a Bader charge analysis, we observe that the Au(111) monolayer gains a small electron charge from graphene and monolayer h-BN. The adsorbed CO molecule adopts similar adsorption configurations on Au(111)/graphene and Au(111)/h-BN with Au-C distance 2.17−2.50 Å and Au-C-O angle of $123.9° - 139.6°$. Moreover, we found that for low CO coverages, bonding to the gold surface is surprisingly energy-favorable. Yet the CO adsorption binding energy diminishes at high coverage due to the repulsive van der Waals interactions between CO molecules.

Lu Wang
Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182

Date submitted: 04 Dec 2012 Electronic form version 1.4