Carbon adsorption on polycrystalline Au surfaces: Orientation dependence of adsorbed work function/dipole moment

HOSSEIN JOOYA, X. FAN, ITAMP, Harvard - Smithsonian Center for Astrophysics, KYLE S. MCKAY, DAVID D.P. PAPPASS, DUSTIN A. HITE, NIST, HOSSEIN R. SADEGHPOUR, ITAMP, Harvard - Smithsonian Center for Astrophysics — We study how the work function due to carbon adatom adsorption is affected by the crystallographic orientation of the gold surface. *Ab-initio* calculations within density-functional theory are performed on carbon deposited (100), (110), and (111) gold surfaces. The work function behavior with carbon coverage for the different surface orientations is explained by the resultant electron charge density distributions. Although the carbon adsorption at sub- to one-monolayer coverage is dictated by different potential energy landscapes of these surfaces, at much higher coverage, all the three orientations would impose approximately the same work function, associated with the work function of the bulk adsorbate, *i.e.* graphite. This systematic study provides a detailed understanding of deposition on polycrystalline gold electrodes which are used in ion microtraps.

Hossein Jooya
ITAMP, Harvard - Smithsonian Center for Astrophysics

Date submitted: 30 Jan 2019
Electronic form version 1.4