

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**First principles study of Bismuth growth on Nickel (111) surface<sup>1</sup>**

QIN GAO, MICHAEL WIDOM, Carnegie Mellon University — A recent experiment (Bollman, et al. 2011) suggests that Bismuth forms flat hexagonally close packed (hcp) films on the Nickel (111) surface, of heights 1, 3, 5 and 7 layers. A quantum size effect (QSE) based on free electrons was proposed in explanation. To test this idea, we calculated the total energy and QSE of Bismuth on Nickel (111) surface using density functional theory. We find the hcp films are destabilized by adding capping atoms which lead to puckering of the hcp layers and covalently bonded structures. Furthermore, we find the rhombohedral films based on the bulk Bi structure are energetically more favorable than the proposed hcp films. These structures also favor odd numbers of layers (a flat wetting layer followed by bulk-like rhombohedral bilayers), but owing to covalent chemical bonding rather than QSE.

<sup>1</sup>Financial support from the ONR-MURI under the grant no. N00014-11-1-0678 is gratefully acknowledged.

Qin Gao  
Carnegie Mellon University

Date submitted: 07 Nov 2012

Electronic form version 1.4