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Bilayer islands in heteroepitaxy of transition metals: insights from first principles[1] TALAT S. RAHMAN, MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, Department of Physics, University of Central Florida, Orlando, FL32816 — Although not in equilibrium configuration, bilayer islands have been observed in the heteroepitaxy of some transition metals for four decades. Its physical origin, however, was investigated experimentally recently for Ru on Pt(111) [1]. By introducing an energy-gain criterion (upon adlayer formation) and by analyzing the density of electronic states of 1 to 3 Ru adlayers on Pt(111), we show that, even though no bonding stronger than that of atoms in bulk Ru is involved, the energy gain for the formation of the second layer is the largest. We find that the effect of the lattice mismatch is not trivial to elucidate from experiment since the electronic structure of a clean substrate changes in the presence of strain and/or chemical bonding with other species. The lattice mismatch, however, is the key factor for the instability in the formation of a third-layer. We extend the model to explain the well-known case of Co/Cu(111) and to predict other possible bilayer systems.

[1] A. Bergbreiter et al., Vacuum **84** 13 (2010)

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Marisol Alcantara Ortigoza
University of Central Florida

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