

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Bonding of adenine on Cu(110) GEOFFREY STENUIT, CNR-INFM DEMOCRITOS Theory@Elettra Group, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy, OKSANA PLEKAN, VITALIY FEYER, KEVIN PRINCE, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy, PAOLO UMARI, CNR-INFM DEMOCRITOS Theory@Elettra Group, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy — We present a density functional study of the adsorption of adenine molecules on the Cu(110) surface. In agreement with experimental core level photoemission and x-ray absorption data, our calculations predict the existence of two phases: a parallel one at low coverage and a perpendicular one at high coverage. These findings resolve contradictions between calculated geometries and published vibrational spectra, and illustrate the complexity of the interaction between a relatively simple bio-molecule and a metal.

Geoffrey Stenuit
CNR-INFM DEMOCRITOS Theory@Elettra Group, Sincrotrone Trieste,
in Area Science Park, I-34012 Basovizza (Trieste), Italy

Date submitted: 02 Dec 2008

Electronic form version 1.4