

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Origin of unexpected attractive adsorbate-adsorbate interactions between negatively charged ions on Mg (0001) surfaces SU-TING CHENG, MIRA TODOROVA, JÖRG NEUGEBAUER, Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — Electrostatic repulsion usually leads to an increase in work function and a decrease in binding energy when the coverage of electronegative elements adsorbed on a metal surface is increased. Using density-functional theory we investigate the adsorption of {N,O,F,Cl} on Mg(0001) and find that only Cl complies with this expectations. All the considered 2nd row elements cause a decrease in work-function and an increase in binding energy with increasing coverage. We show that these counterintuitive phenomena can be understood in terms of an efficient embedding of the adsorbate atoms into the unusually large electronic surface spill-out of Mg(0001). The described mechanism is based on purely electrostatic arguments and thus expected to be a generic feature on surfaces consisting of highly electropositive elements.

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Date submitted: 13 Nov 2013

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