

A DFT study of the adsorption of Au on Ni(111)

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Abstract

Recent experimental STM studies for the adsorption of Au/Ni(111) display a broken symmetry in the obtained STM pictures. Therefore, we have studied the adsorption phenomena of Au on Ni(111) using the Density Functional Theory, employing a plane wave basis set. To solve the Kohn-Sham equations, we have used the Vienna ab-initio simulation package (VASP)^{1,2,3}.

We have concentrated on the investigation of the structural and electronic properties of the system. The system has been modeled by four layers of Ni with nine atoms per layer forming a p(3x3) superstructure (resulting in a coverage of Au of about 0.11ML), separated by a vacuum layer more than 30 Å. In all cases, the two topmost Ni layers were allowed to relax. Brillouin zone integrations have been performed using a 5x5x1 Monkhorst-Pack grid⁴. We have investigated an adsorption of Au in the high-symmetry sites; i.e. the top, bridge and fcc/hcp hollow positions. We found that the fcc hollow position is favored from an energetic point of view. Calculations for a higher coverage, resulting in a p(2x2) superstructure, lead to the same results.

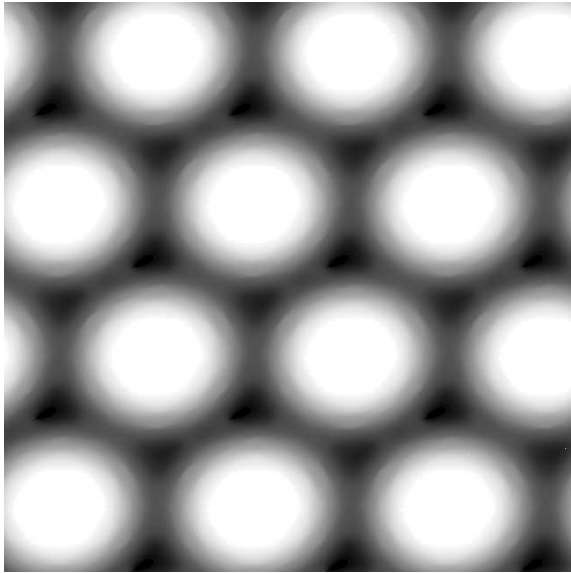
An analysis of the density of states (DOS) allows a characterization of the electronic properties of the adsorption. The adsorption is determined by an interaction of the Ni d_{yz} , d_{xz} and d_{z^2} with the Au d-orbitals. Furthermore, the experimental STM pictures will be confronted with pictures simulated from our calculations.

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Pic 1. Simulated STM picture (constant current) for Au 0.11ML on Ni(111). The picture is simulated with a bias voltage of 0.4 eV for the hcp hollow position.

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