ATOMIC STRUCTURE AND ELECTRONIC PROPERTIES OF Pb/Mo(110) SYSTEM

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We present theoretical study of the atomic structure and electronic properties of Pb/Mo(110) system. In the first step we performed surface relaxation of clean Mo(110) substrate. Interatomic distances, electronic structure, surface energy and work function have been compared with the corresponding results provided by the previous ab-initio calculations. Adsorption of Pb was considered for the coverage of 0.25 ML. For this coverage we have found three stable adsorption points of Pb atom. We have presented detailed analysis of the atomic configuration, electronic structures and adsorption energies in these three cases.
Our results will be also considered in the context of existing experimental data.

LOCAL ELECTROSTATIC FIELDS NEAR THE CARBON SURFACE: FIELD-INDUCED ELECTRON DENSITY REDISTRIBUTION

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The application of supersonic helium beams for the beam-surface and beam-cluster scattering experiments stimulates the interest to the spatially-resolved neutral particles detection. The field ionization may provide the high detection efficiency and the spatial resolution on a nanoscale. Especially the carbon nanotubes and nanotips serving as field-ion emitters seem to be promising in this aspect since they can be arranged in the arrays containing millions of emitters providing thus the necessary density of the detecting elements. However, while the field ionization over the metal surface has received lot of theoretical attention in recent years, the field-induced processes at a carbon nanotube surfaces are almost not considered theoretically.
Therefore, such theoretical tasks as the local field distributions, estimates of field penetration into the bulk, induced-surface-charge distribution, location of the effective charged surface and the screening length are topical problems urgently waiting for the thorough and detailed studying.
In the present contribution a new approach is proposed for the calculations of the field-free and field-modified electron density distributions at the surface of a semi-infinite carbon crystal using the functional integration method [1]. This allows a correct consideration of the exchange-correlation effects and makes possible the calculations of the local electrostatic fields near the carbon surface (of the order of volts per angstrom) without to use the perturbation theory.

[1] P.P. Kostrobiy, B.M. Markovych, Condens. Mat. Phys. **6**, (2003) 347.