Oxygen Adsorption on the Be-covered Mo(112) Surface: DFT Study

Afanasieva T.V.[1], Petrova N.V.[2], Yakovkin I.N.[2]

[1] *National Taras Shevchenko University of Kyiv, Kyiv, Ukraine*
[2] *Institute of Physics of National Academy of Sciences of Ukraine, Kyiv, Ukraine*

It has been shown that both on a clean and (1×1)Be-covered Mo(112) surface, oxygen will readily dissociate, without any noticeable barrier, and the presence of Be in the furrows rather facilitates than hinders the dissociation. The O_2 molecules can be adsorbed also on Be rows in several metastable configurations, which can be considered precursor states for the dissociation. The O atoms will occupy bridge-on-row sites, which remain available for oxygen in presence of the (1×1)Be monolayer, because Be atoms occupy adsorption sites in furrows. However, the co-adsorbed Be – O monolayer is found to be unstable (or metastable). In particular, O atoms, being slightly shifted from the symmetrical position in the bridge-on-row sites, tend to move towards Be atoms and spontaneously form Be_2O or, at higher oxygen exposures, BeO, which is consistent with recent AES studies for this system. The estimated gain in energy due to reaction of the BeO formation on the Mo(112) surface is of 1.17 eV. At lower oxygen coverages, the formation of Be_2O is more favorable (by 0.15 eV) than the configuration of BeO with some non-oxidized Be adatoms on the surface.