

Structure of MgO and CaO(100) surfaces and their Interaction with Representative Metal Adsorbates. *Dominic Alfonso, James Snyder, John Jaffe, Anthony Hess and Maciej Gutowski. Pacific Northwest National Laboratory, Richland, WA 99352, USA.*

All- electron Density Functional Theory calculations using periodic slab approach are carried out to investigate the relaxed structures of the regular MgO and CaO(100) surfaces and their interaction with alkali metals (Li and Na). For MgO, the cations are displaced downwards relative to the oxygens whereas the relaxation pattern is opposite in the case of CaO. For a given alkali atom and coverage, the interaction energy between the oxide slab and the metal net is larger for CaO. The lateral interaction among adsorbed alkali atoms contributes significantly to the stabilization of the metallic layer. The 1.0 ML of Li is found to be energetically stable with respect to the formation of a three dimensional island and the small lattice mismatch between the MgO substrate and bcc bulk Li suggests that formation of low energy interface may occur between these two materials. We also present interaction of Cu with the CaO(100) substrate. Our results provide theoretical evidence for the formation of c(1x1) Cu layer on CaO.