E2-01 : HYDROGEN ADSORPTION ON THE Be(0001) SURFACE : A QUANTUM CHEMICAL STUDY

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An ab initio Hartree-fock crystal orbital study to model H adsorption on the Be(0001) surface at different coverages is presented. Both single (1L) and triple (3L) layer Be slabs with H on one of the four possible high symmetry sites, on-top,bridge, three-fold open and eclipsed are considered. The bonding geometry, binding energy and fundamental vibrational frequencies for the three H coverages (0.25, 0.5 and 1.0) on Be (0001) have been calculated. At 0.25 monolayer (ML) coverage, the energetically most preferred site for the H adsorption is an on- top site. When the coverage is increased to 0.5 ML H. prominent changes to the binding energy appeared. Energetically, the most favoured site is the bridge site and the open site is 8.5 KCal/mol above the bridge site. This agrees with electron energy loss spectroscopy (EELS) experiments which assign H atoms to bridge sites when there is low surface coverage (0.38 ML H). The Be - H equilibrium bond length is decreasing with the increasing H coverage for all three sites considered. Calculated vibrational frequencies at the three coverages for three sites fall into the same trend where the energy of the Be-H stretch decreases with increasing adatom coordination.