First-principles study of ammonia synthesis on a supported iron nanocluster

ZELJKO SLJIVANCANIN, Institut Romand de Recherche Numerique en Physique des Materiaux, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland, ALFREDO PASQUARELLO, Institut Romand de Recherche Numerique en Physique des Materiaux, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — Possibility of ammonia synthesis on a MgO(100) supported iron nanocluster has been studied using density functional theory. The $N_2$ molecules were sequentially adsorbed on the $Fe_7/MgO(100)$ and the most favorable adsorption geometries and dissociation pathways investigated. The first two $N_2$ molecules were found to dissociate easily upon adsorption, producing nitrogen atoms which bind strongly to the cluster. The third $N_2$ molecule adsorbs in a favorable molecular state without dissociating. Adding H atoms one by one to the adsorbed $N_2$ molecule we found that two H atoms are required to break the molecule and then, after adding another two H atoms, the first ammonia is formed. The process is accompanied with a small energy barrier and the microscopic mechanism is similar to the one proposed for the biological nitrogen fixation.