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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.

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