

Abstract Submitted  
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**Stabilization of Reactive MgO Surfaces by Ni Doping**<sup>1</sup> ALIAKSEI MAZHEIKA, SERGEY V. LEVCHENKO, Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — Ni-MgO solid solutions are promising materials for catalytic reduction of CO<sub>2</sub> and dry reforming of CH<sub>4</sub>. To explain the catalytic activity, an *ab initio* study of Ni-substitutional defects in MgO (Ni<sub>Mg</sub>) has been performed. At first, the validation of the theory level was done. We compared results of CCSD(T) embedded-cluster calculations of Ni<sub>Mg</sub> formation energies and adsorption energies of CO, CO<sub>2</sub> and H<sub>2</sub> on them to the HSE( $\alpha$ ) hybrid DFT functional with the fraction of the exact exchange  $\alpha$  varied between 0 and 1 [1]. HSE(0.3) was found to be the best compromise in this study. Our periodic HSE(0.3) calculations show that Ni<sub>Mg</sub> defects are most stable at corner sites, followed by steps, and are least stable at (001) terraces. Thus, Ni-doping stabilizes stepped MgO surfaces. The dissociative adsorption of H<sub>2</sub> on the terrace is found to be endothermic (+1.1 eV), whereas on (110) surface with Ni<sub>Mg</sub> it is highly exothermic (−1.6 eV). Adsorbed CO<sub>2</sub> is also significantly stabilized (−0.6 vs. −2.2 eV). These findings explain recent microcalorimetry measurements of H<sub>2</sub> and CO<sub>2</sub> adsorption at doped Ni-MgO samples.—[1] A. Mazheika and S.V. Levchenko, DOI: 10.1021/acs.jpcc.6b09505.

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