ADSORPTION OF WATER ON MgO NANO-STRUCTURED SURFACES IN THE PRESENCE OF DEFECTS, DOPANTS AND VACANCIES

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We have used density functional at the b3lyp/6-31g* level to investigate the adsorption of water, with relaxation at low coordination sites of nanostructures containing defects (kinks, steps, terraces, corners, edges) , dopants (K, Li, Na, Al, Ca, ……) and vacancies (F centers) in order to investigate binding energies of adsorption, charge distribution, bonding parameters and energy gaps. Our results indicate that the physical-chemical parameters investigated are very sensitive to defects , dopants, coordination sites as well as oxygen vacancies of our MgO nanostructures.

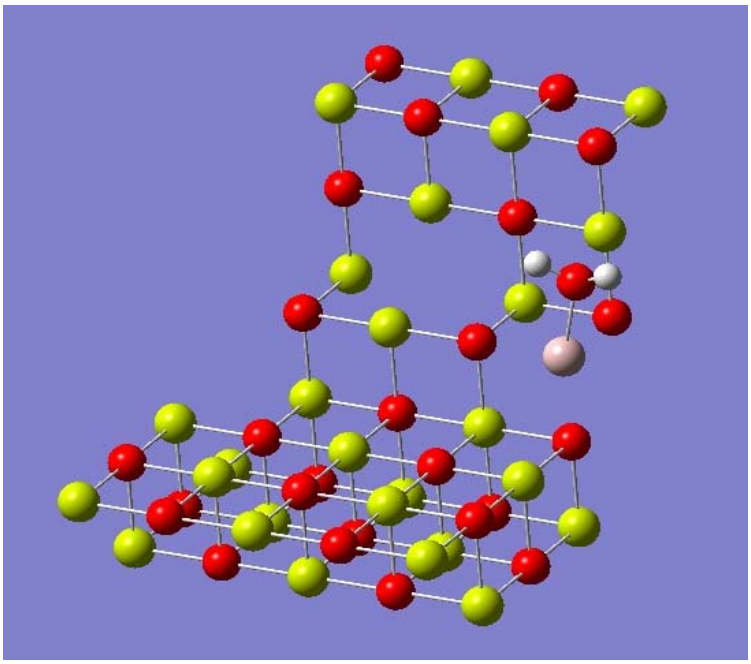

Fig.1. Adsorption of water at positions with dopants, defects, and vacancies of MgO.

References:

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