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

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Heteregeneous catalysis at surfaces is important industrially, environmentally and biologically. We have investigated the dissociation of water on low coordination sites nano-structured surfaces of MgO in the presence of defects (kinks, steps, terraces, corners, edges..), dopants (K, Li, Na, Al, Ca, V, Cr, ……) and vacancies (F color centers) using density functional at the b3lyp/6-31g* level and taking relaxation effects into consideration as well, in order to investigate dissociation energies, (MgOH and OH binding parameters), charge distribution, reaction pathways, and energy gaps. Our results indicate that the physical-chemistry parameters investigated are very sensitive to relaxation of the cluster, defects, dopants, coordination sites as well as oxygen vacancies of our MgO nanostructures.

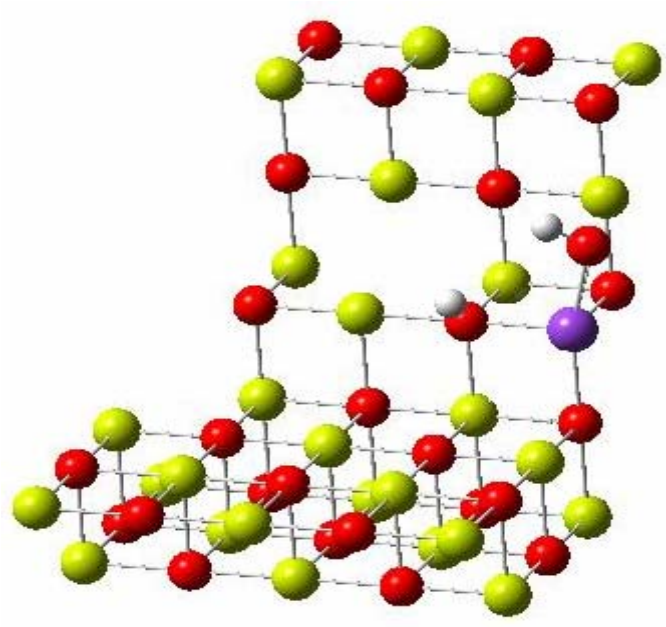

Fig.1. Water dissociation

References:

1. **A. L. Almeida, J. B. L. Martin, C. A. Taft, E. Longo & W. A. Lester. Jr, Int. J. Quantum. Chem. 71, 153 (1999).**

2. **A. L. Almeida, J. B. L. Martins, C. A. Taft, E, Longo, W. A. Lester Jr., J Chem Phys 109, 367, 1998.**

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