Department of Physics (Autonomous) University of Mumbai
Ph.D. Seminar
of

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Design and development of low-cost materials for application in photocatalysis and hydrogen storage

The present thesis addresses two major issues of energy and environment. First section focuses to identify new materials for H_2 storage application using density functional theory (DFT). Hydrogen fuel is one of the most promising alternatives to conventional energy sources as it is abundant, environment friendly and has the highest energy density. However, the efficient and compact hydrogen storage is a major challenge for practical implementations of hydrogen fuel. Solid state storage would be most efficient method if it can be able to achieve the US Department of Energy (DoE) prescribed the guidelines that it should be able to store a minimum of 5.5 wt % of hydrogen by weight, with binding energy in the range of 0.1−0.7 eV. DFT calculation of 2D Cr_2C layer and Zr decorated graphene suggests it can be able adsorb 6.4 and 11 wt%of H_2 with average binding energy (BE) 0.33 and 0.34 eV/H_2 which is greater than the 2017 DoE recommended target value of 5.5 wt.%. This study also reveals for the first time, dependency of desorption temperature (T_D) of H_2 molecule with the magnetic moment (μ) of the system following an empirical relation $T_D = T_0 + a\mu^b$ (with T_0 = 399K, a = 302.38 $J^{-1}TK$ and b = 0.5).

The second part of the thesis focuses on development of efficient photocatalyst materials for photocatalytic degradation of industrial waste (phenol). For photocatalytic application, the efficiency of TiO_2 is limited due to its wide bandgap, which restricts light absorption within UV range (5% of solar spectrum), and high bulk and surface recombination rates of the produced electron-hole pairs. Combining TiO_2 with reduced graphene oxide rGO has shown great improvement in the photocatalytic activity in this field by huge reduction in surface recombination rate via electron transfer from TiO_2 to rGO through Ti-O-C bond formed at interface of composite. .Reduction of rate of recombination can be controlled by varying GO to TiO_2 weight ratio, which should be optimized in order to obtain efficient photoctalyst. rGO-TiO_2 composites are prepared using photo-reduction method by varying GO to TiO_2 weight ratio and its effect on morphological, optical and mechanism of fast charge dynamics at the interface are investigated. The experimental findings were further investigated using density functional theory simulations. Band structure calculation confirms high mobility states induced within the band gap due to formation of Ti-O-C bond in rGO-TiO_2 model which assists in fast electron transfer from TiO_2 to rGO during the photocatalytic process and hence reduces recombination rate.

Wednesday 13th April, 2019
at
Seminar Hall, Department of Physics, 3rd floor,
Tilak Bhavan.
Time: 14.30hrs

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