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Theoretical and Computational Study For Ferroelectric Photocatalysts

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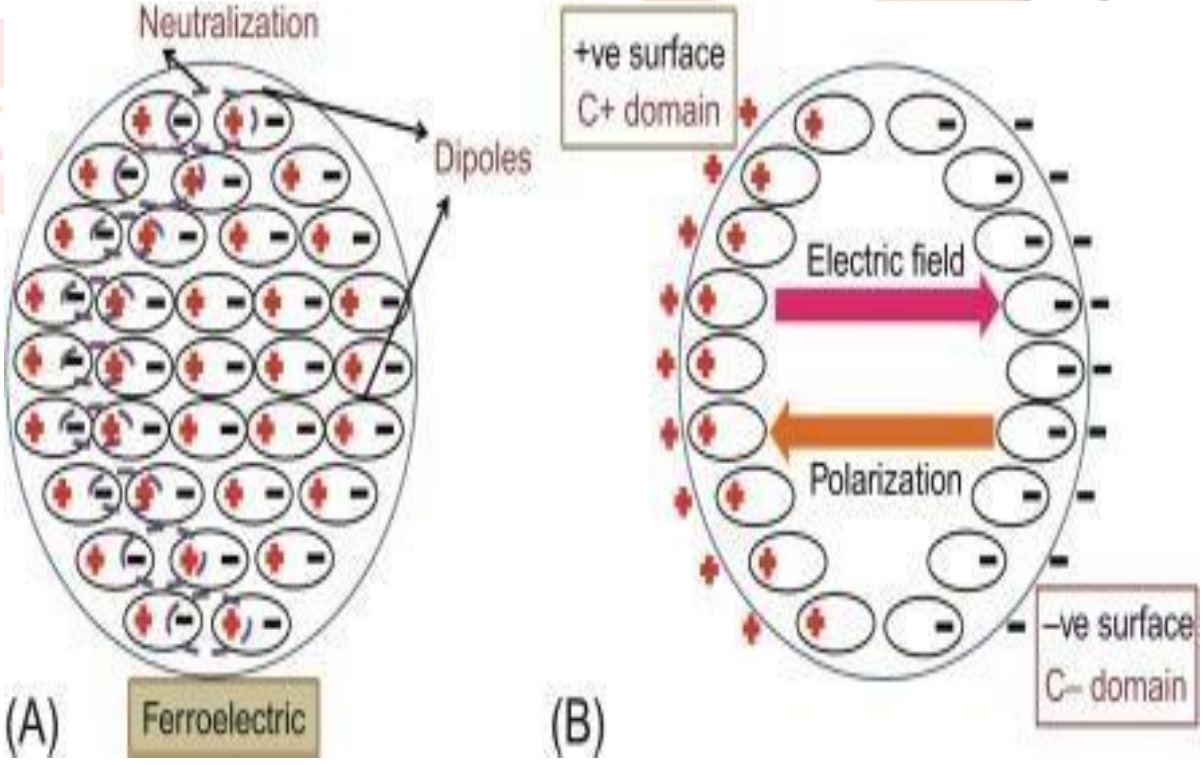
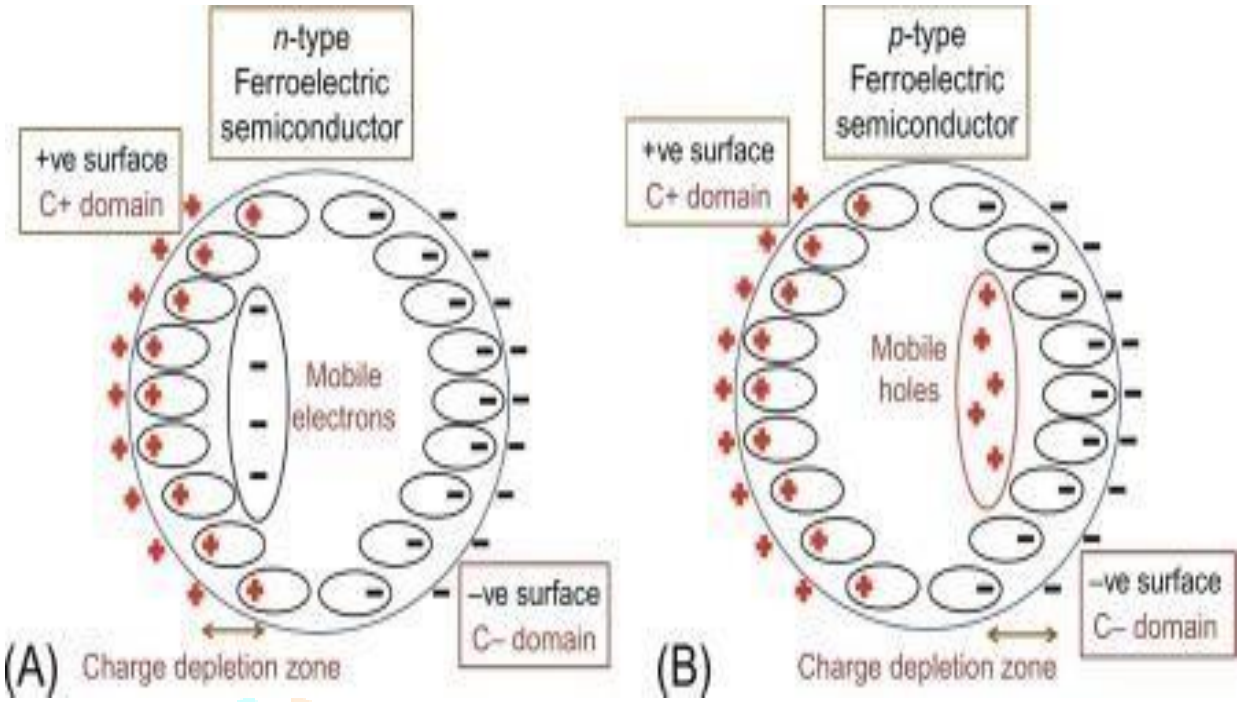
The theoretical simulation and computational method are proposed to identify the in fundamental physical properties of ferroelectric semiconductors, in particular the correlation between their composition , structure and electrical properties. Emerging ferroelectric materials greatly developed the prospect of using sunlight for environmental and energy purpose. This paper presents the fundamental and importance of spontaneous polarization and induced electric field formation in ferroelectric semiconductor materials advantage for photocatalytic activities. In this paper addresses the process of obsorption and spatially selective oxidation/reduction reactions. In this paper also addresses the issue of effectively detective the photo-generated electrons and holes which is also evidently essential to improve the the photocatalytic activity of semiconductors.

Keyword:- Ferroelectric Photo catalysts, Photo-generate.

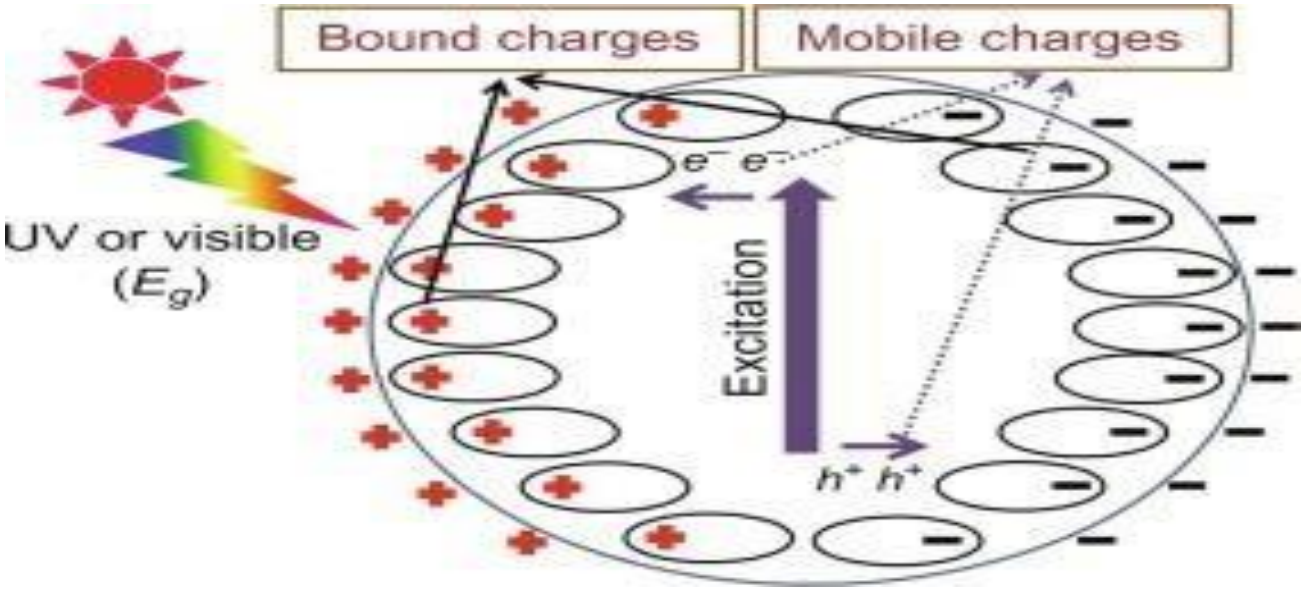
The theoretical simulation in computational method are introduced to identify the fundamental physical properties of ferroelectric semiconductor, especially the correlation between their composition and structure and electrical properties. Theoretical methods play a promising a role in prudently predicting the electronic structure and charge distribution in catalytic materials. First principle computational methods are widely used in this study of ferroelectric preovkite-type oxides. This methods have extended the theoretical knowledge

and sensibility of these materials. The first principle density functional theory (DFT) calculations have effectively facilitated our current understanding of fundamental insight such as the origins of ferroelectricity in oxides, which in turn led to appropriate understanding of electronic hybridization topology and mechanism by predicting the material and environmental+specific properties of ferroelectrics. First principle method are generally used because they know only on parametrize theories and because they can be fitted to potentially inaccurate experiments. They can be applied to materials that are not yet synthsized and temperature, pressure or compositions for which data are not available. Instead of experimental data constraint parameters. We must start from the fundamental interaction among electrons and nuclei. Most of the first principle method that have been applied to ferroelectrics are based DFT, through some are based on the Hetree -Fock theory. The DFT method computers the ground state properties of a system with the charge density and utilizes the effective charge correlation potential (Vxc) to compute the quantum mechanical interaction between the electron charge density and energy distribution.





The local density approximation (LDA) take the Vxc from the uniform electron gas as the density for each point in the materials. The generalized gradient approximation(GGA) includes the effect of local gradient in the density. We can find the effective potential of Hamiltonian fitting from the first principle results in obtaining finite temperature properties using Monte-Carlo or molecular dynamics method for last systems. The first principles computational method is cost effectively and applicable to more materials and systems than the recent experimental methods, which are more accurate highly sensitive costly and largely dependent on the quality of samples. In One dimensional (1D) nanostructures, it is possible to enhance the photoreactivity by tunning the transport of photogenerated charge carriers throught quantum confinement. Zhang et al. discover between ferroelectric polarization and electronic structure in photoreactivity enhancement with the help of spin-polarized DFT calculations using CASTEP programs, which accounted for the prominent reactivity of O- KNbo3 as compared with m- KNbo3.


Bound charges
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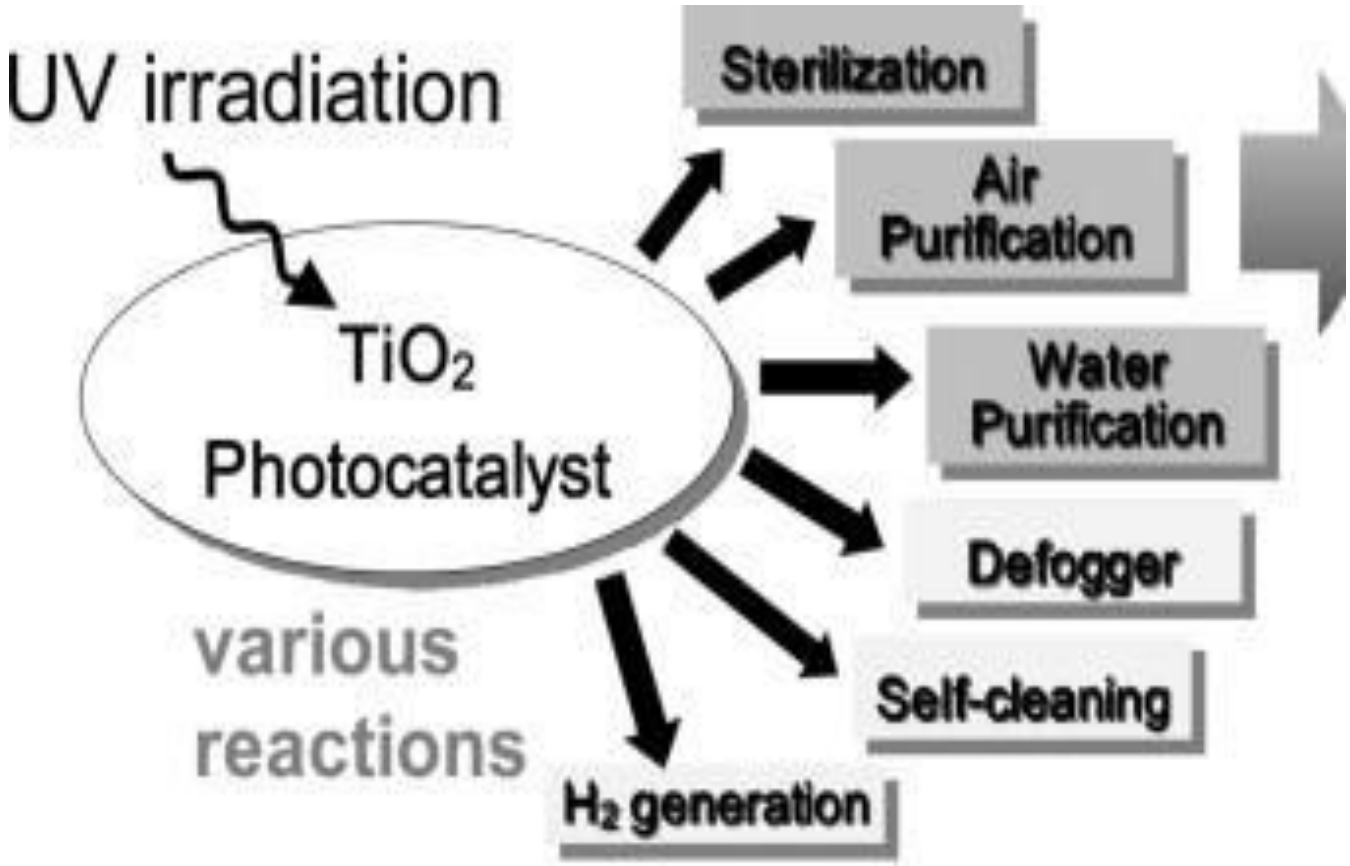

From the first principle method is is concluded that the polarization rotation tends to reduce the band gaps of strongly distorted preovkite. Various visible light ferroelectric salt solution are designed by Wang et al. by incorporating Zn into KNbo3. In theoretical calculation, Alkeisy et al. found excellent Photocatalytic performance is highly ferroelectric Ag10 Si4O13. Using the Vienna Ab- initio simulation package (VASP) best on DFT with the projector arugmented wave (PAW) pseudo potential method and hybrid functional calculations they simulated ferroelectricity originating from an anisotropic and highly dispersive band structure of Ag10Si4O13 due to its p-block electronic configuration. They found that intrinsic internal E was induced in Ag10Si4O13 due to the long distorted SiO4 chains, which further enhence the Photocatalytic activity by effective separation of photo induced charges.

Using first principle calculation, Xu et al. found that in two dimensional materials monolayer AgBiP2Se6 which exhibits the out plane ferroelectricity having a thinkness of only 6 angstrom out-plane polarization could enhance the e^- and h^+ separation and thus AgBiP2Se6 can be used as visible light photocatalysts for water splitting. Glickstein et al. developed a quantitative One

dimension and two dimension COMSOL computational model for the heterostructured ferroelectric Photocatalysts to predict the photocatalytic performance of TiO2 flims on ferroelectric BaTiO3. Simulation showed that the internal quantum efficiency(IQE) could be increased more than 90% by controlling key parameters, including the domain width, increasing the reduction reaction kinetics; increasingly the career life time; and optimising the potential use in models are very accurate for studying finite temperature properties of ferromagnetic.

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