# Realization of the role of donor (F) impurity on the electronic structure and optical properties of ZnO: A first principles study

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## Abstract

We perform first principles calculations based on density functional theory to investigate the effect of F doping on the electronic and optical properties of ZnO. Electronic band structure study confirms the degenerate semiconducting nature with n-type conductivity in pristine ZnO and as well in F-doped ZnO. The increase of band gap in F: ZnO is attributed to the well-known Burstein-Moss effect which is in accord with experimental results. Furthermore, it is elucidated that incorporating F into ZnO introduced impurity bands below the conduction band (CB), subsequently, the Fermi level shifted towards CB. The shifting of Fermi level into CB fallouts the improvement of electrical conductivity and carrier concentrations of the doped system. Different optical properties such as dielectric constant, optical absorption, reflectivity, photoconductivity, refractive index and dielectric loss function have also been studied as a function of photon energy. The absorption spectra of F:ZnO approved that the blue shift occurs at the absorption edge. This result implies that the optical band gap has increased which complies with the electronic study. These findings suggested that F doped ZnO system could be a potential candidate for short wavelength optoelectronic and photo-electrochemical applications.

## Introduction

- ZnO is a cheap and nontoxic n-type semiconductor.
- Wide band gap 3.37 eV and large exciton binding energy 60 meV.
- Easy to fabricate using cost effective process.
- High optical transparency.
- Doping enormously changes the physical properties of ZnO.
- Extensively used in spintronic, TCOs, transistors, diluted magnetic semiconductors, DSSCs etc. [1]
- Investigation of the effect of F doping on ZnO is prime goal of the present work.

## Computational Details

- ✓ CASTEP code [2] was used for the DFT based first principles calculations.
- ✓ GGA –PBE was used for the exchange-correlation potentials.
- ✓ Ultrasoft pseudopotential describe the electrons and core interaction.
- ✓ The 2x2x2 supercell contains 32 atoms.
- ✓ The plane-wave cutoff energy=480 eV, and a Monkhorst-Pack scheme with 5×5×3 k-points were implemented for Brillouin zone sampling.
- ✓ Optimize structure was used to calculate electronic and optical properties of un-doped and F-doped ZnO.

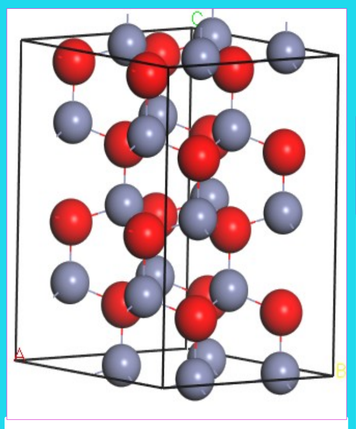

Fig. 1: Crystal structure of ZnO.

## Results and Discussions

Table: Optimize lattice parameters (*a* & *c*) (Å), *c/a* ratio, volume, V and band gap, $E_g$ (eV) of ZnO and F:ZnO.

| $ZnO_{1-x}F_x$ | *a* | *c* | *c/a* | V | $E_g$ |
|---|---|---|---|---|---|
| x = 0.0 | 3.294<br>3.295 [3] | 5.298<br>5.290 [3] | 1.606<br>1.605 [3] | 49.63<br>49.61 [3] | 0.73<br>0.74 [3] |
| x = 0.0625 | 3.316 | 5.350 | 1.613 | 50.75 | 1.79 |
| x = 0.125 | 3.338 | 5.404 | 1.619 | 51.83 | 2.69 |

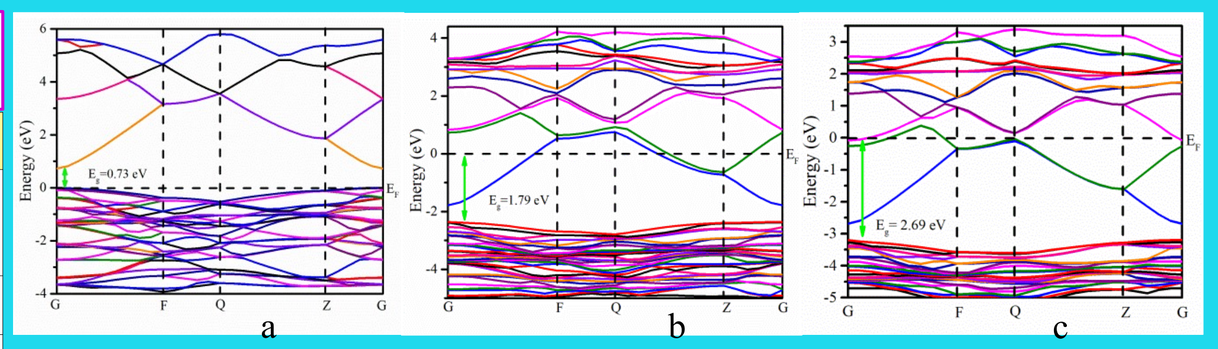


Fig. 2: Electronic band structure of $ZnO_{1-x}F_x$ a) x=0, b) x=0.0625 c) x= 0.125

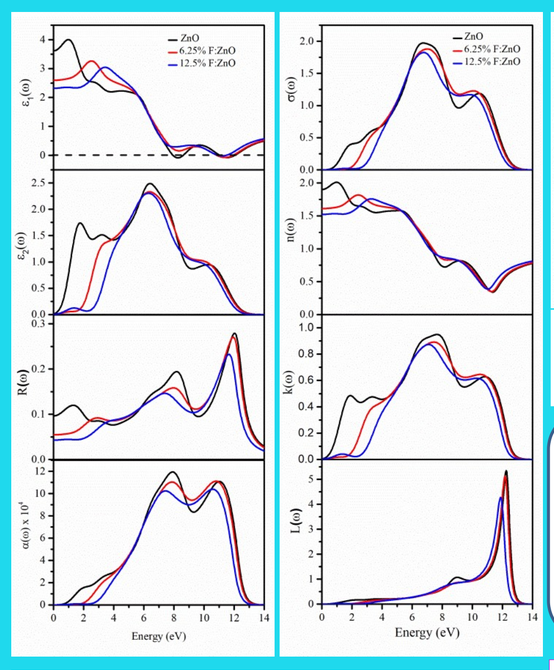


Fig. 4: Optical properties of ZnO and F:ZnO

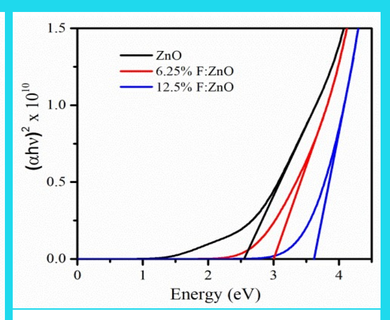


Fig. 5: Optical band gap of ZnO and F:ZnO

- ❖ Blue shift at absorption edge
- ❖ Burstein-Moss effect
- ❖ High conductivity

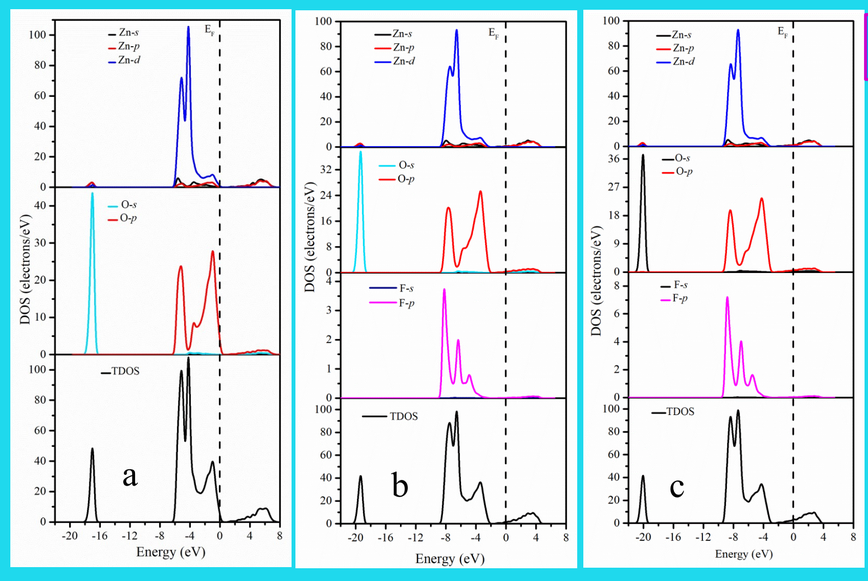


Fig. 3: DOS of $ZnO_{1-x}F_x$ a) x=0, b) x=0.0625 c) x= 0.125

## Conclusions

- ➢ Optimized lattice parameters are agreed well with available data.
- ➢ Impurity states introduced below C.B.
- ➢ Band gap increased for F doping into ZnO due to B-M effect.
- ➢ n-type conductivity with enhance carrier concentration.
- ➢ Enhanced optical band gap of F:ZnO.
- ➢ Transmittance will be higher than that of ZnO.
- ➢ Suitable for optoelectronic device applications.

## References

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