Enhancing N-Type Conductivity in ZnO through Chlorine and Fluorine Doping: Hybrid Functional Calculations

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Zinc oxide (ZnO), a wide-bandgap semiconductor, is widely recognized for its optoelectronics applications, such as ultraviolet lasers, light-emitting diodes, and liquid crystal displays.[1] In this study, we investigate the effects of halogen doping, specifically chlorine (Cl) and fluorine (F), on enhancing carrier concentration and improving n-type conductivity in ZnO through hybrid density-functional (HSE) calculations. The predominant configurations and the electronic properties of the Cl and F impurities are determined through the calculated formation energies. Unlike previous reports,[2,3] we find that both the substitutional Cl_O and F_O act as shallow donors. Under the O-poor condition, Cl_O and F_O are the most energetically favorable for the Fermi-level values near the conduction band minimum. This indicates that these defects can significantly increase electron concentration and enhance n-type conductivity. Moreover, the formations of complex defects between the halogen impurities and the native defects are investigated to provide a deeper understanding of their impact on the defect chemistry of ZnO. This work offers valuable insights for optimizing *n*-type conductivity in ZnO and contributes to the development of future optoelectronic devices.

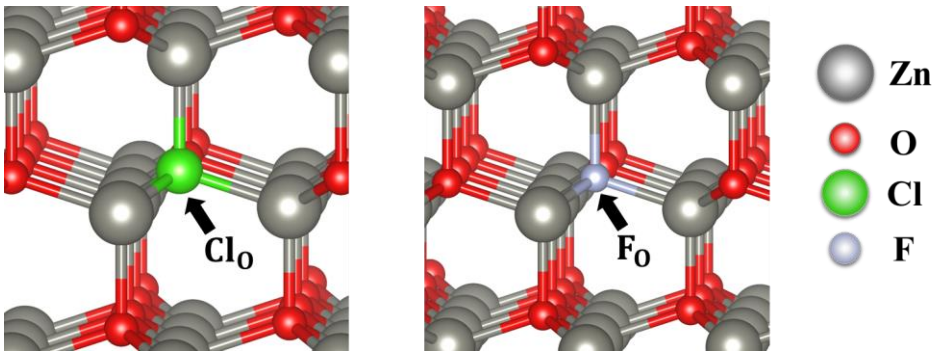

Figure 1 Local atomic structures of (a) Cl_O and (b) F_O in ZnO. The grey, red, green and light blue spheres represent Zn, O, Cl and F atoms, respectively.

References

1. Janotti, Anderson, and Van de Walle, Chris G. Physical Review B, **200**7 16, 165202.
2. Liu, Bo, *et al*. Applied Physics Letters, 2010, 97, 12.
3. Liu, Bo, *et al*. Solid state communications, 2013, 171, 30-33.