Defects and Doping in $ZnGeN_2$

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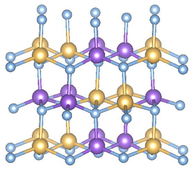
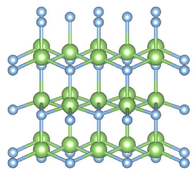
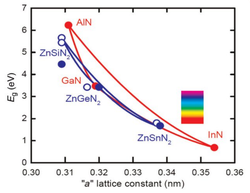
Motivation



Orthorhombic $ZnGeN_2$



Wurtzite GaN

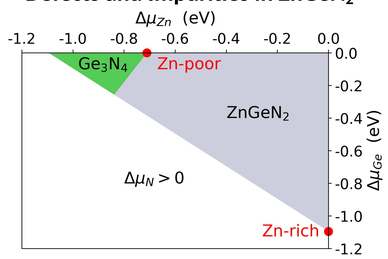


Quayle, P.C., *et al.*, MRS Comm., 3(3), 135–138. (2013).

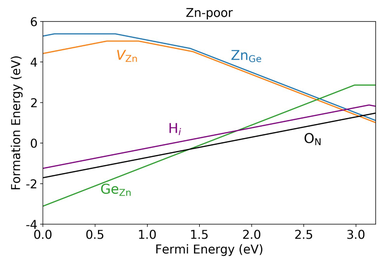
- II-IV-nitrides are a promising class of materials formed from earth-abundant materials that exhibit a wide range of band gaps and spontaneous and piezoelectric polarization moments.
- Potential for optoelectronic and electronic devices.
- Orthorhombic II-IV-nitride unit cell derived from cation mutation of wurtzite III-nitrides: group III → group II + IV
- **What are the properties of defects and prospects for controlled doping in these materials?**

Native point defects and impurities in $ZnGeN_2$

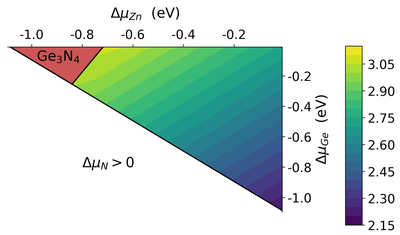
Defects and Impurities in $ZnGeN_2$



Defects and Impurities in $ZnGeN_2$



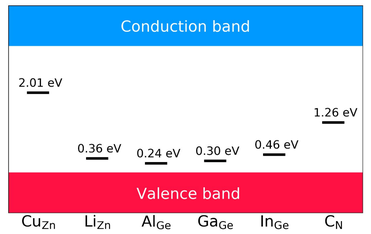
Variation in Fermi-level pinning due to O_N and Zn_{Ge}



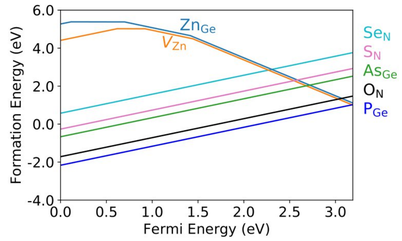
- Oxygen and hydrogen are donors in $ZnGeN_2$, strong compensation by vacancies (V_{Zn}) and antisites (Zn_{Ge})
- Fermi level is closest to the CBM (3.19 eV) under Zn-poor conditions.

Candidate *p*-type and *n*-type dopants in $ZnGeN_2$

Acceptor levels due to substitution on Zn, Ge, and N sites



Formation energy of candidate donors

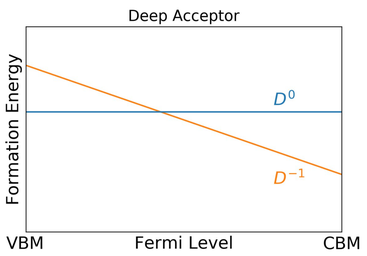


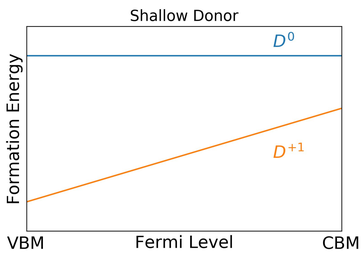
- All candidate acceptors have transition levels within the band gap
- Al_{Ge} has a transition level 0.24 eV from the VBM; similar to Mg in GaN
- All candidate donors are shallow
- P_{Ge} has the lowest formation energy, and least risk of compensation

Methodology

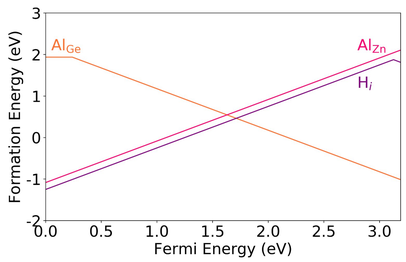
- Density functional theory with the Heyd-Scuseria-Ernzerhof[1] functional implemented in VASP[2]
  [1] J. Heyd, G. Scuseria, M. Ernzerhof, J. Chem. Phys. **124**, 219906 (2006)
  [2] G. Kresse and J. Hafner, Phys. Rev. B **54,** 11169 (1996)
- Defect formation energies calculated using a 128-atom supercell with electronic corrections.
  C. Freysoldt *et al.*, Phys. Status Solidi B 248, 1067 (2011)

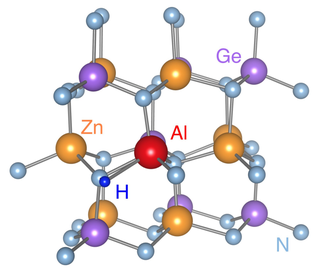
Deep versus shallow defects





Hydrogen-assisted *p*-type doping

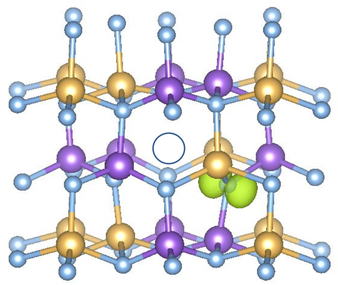




- Al incorporates on Ge and Zn sites
- → strong compensation → limits *p*-type doping by Al_{Ge}
- Al_{Ge} forms neutral complexes with H similar to Mg_{Ga} – H in GaN
- Al_{Ge} – H binding energy calculated to be 0.55 eV
- Diffusion barrier for H in $ZnGeN_2$ is 1.2 eV
- H can be removed in a post-growth anneal

Conclusions

- Native point defects in $ZnGeN_2$ lead to insulating material.
- Al_{Ge} can lead to *p*-type doping in $ZnGeN_2$.
- H-assisted doping increases Al substitution on the Ge site.
- P_{Ge} is a promising *n*-type dopant.



This work was supported by the Army Research Office (ARO) under grant number W911NF-16-1-0738. Computational resources were provided by CNSI/MRL, NERSC, and XSEDE.