Supplementary Information

Zinc Germanium Nitrides and Oxide Nitrides: The Influence of Oxygen on Electronic and Structural Properties.

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1. DOS Figures $ZnGeN_2$

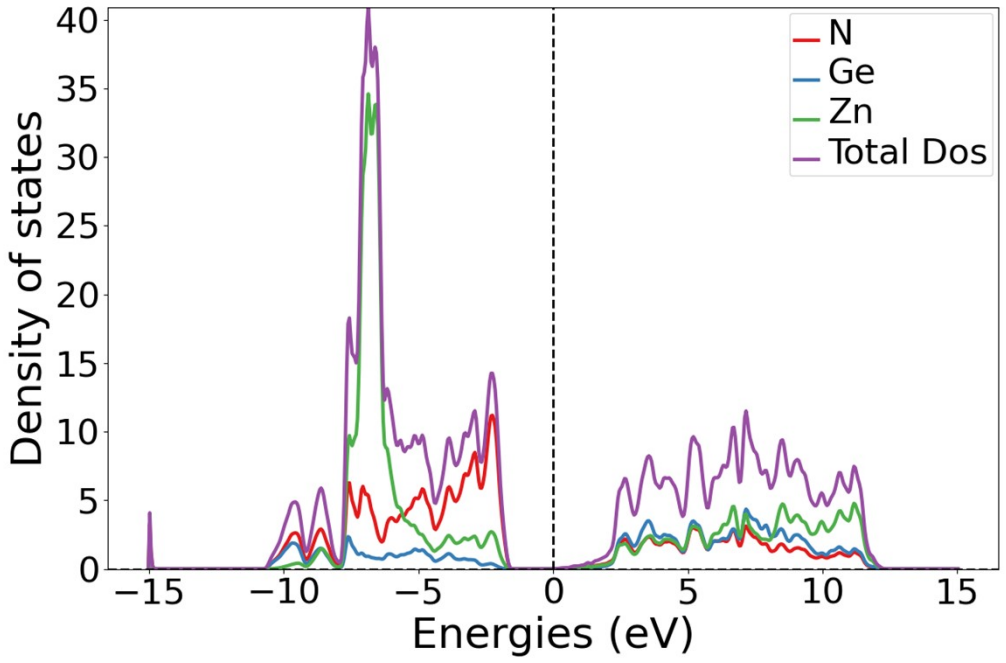

Figure S1: DOS of ZnGeN2 with pDOS of the different atom types.

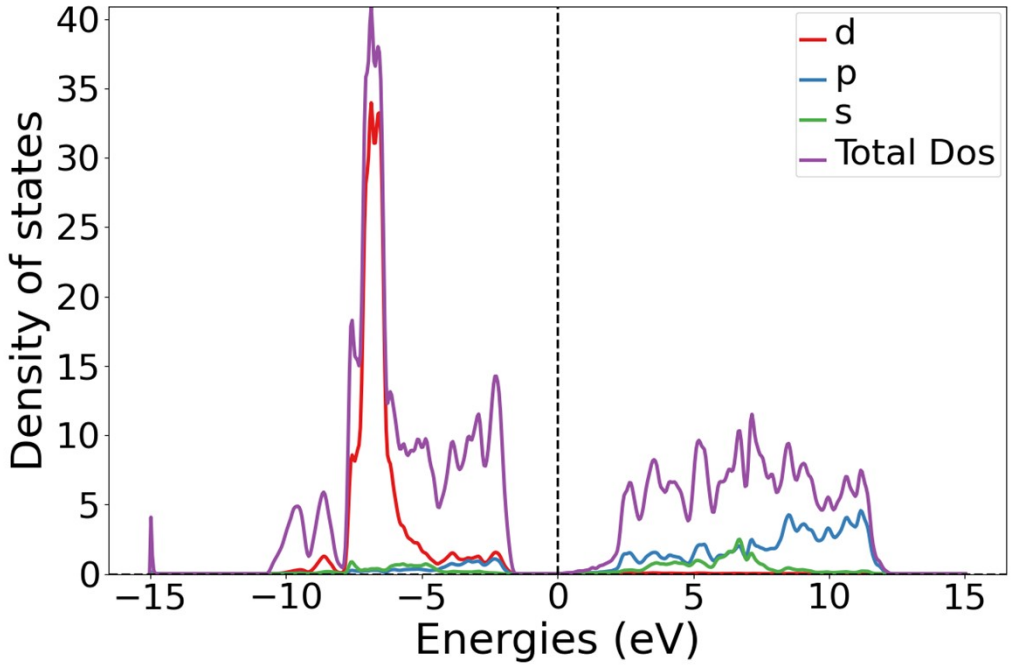

Figure S2: Orbital separated pDOS of the Zn orbitals

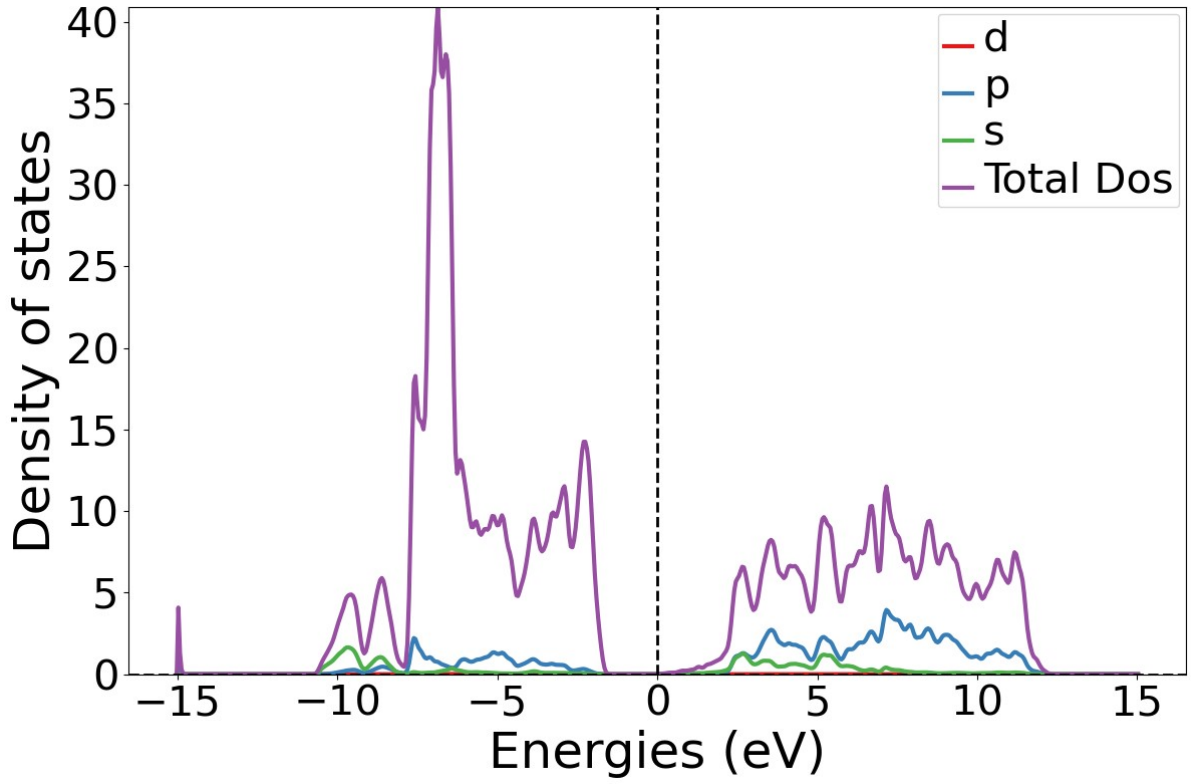

Figure S3: Orbital separated pDOS of the Ge orbitals

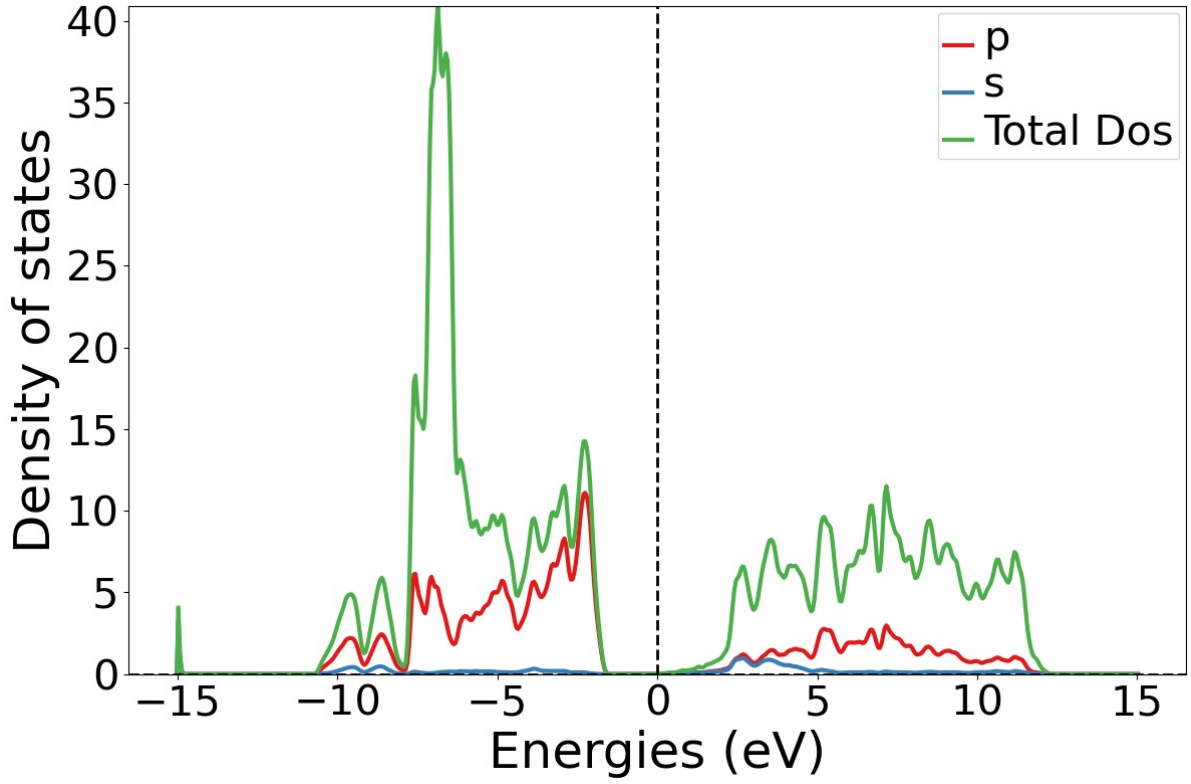

Figure S4: Orbital separated pDOS of the N orbitals

2. DOS of $Zn_{1.25}Ge_{0.75}(N_{0.75}O_{0.25})_2$ (a)

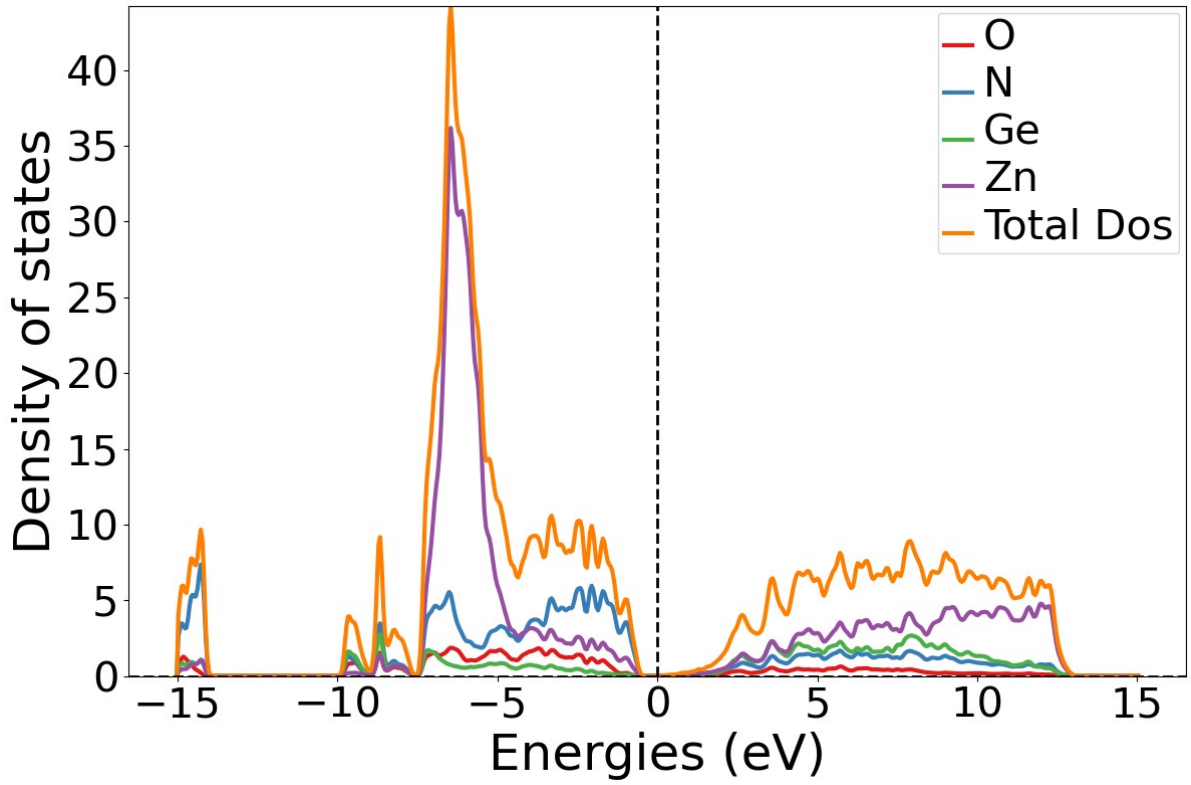

Figure S5: Total DOS with pDOS contributions of all atom types.

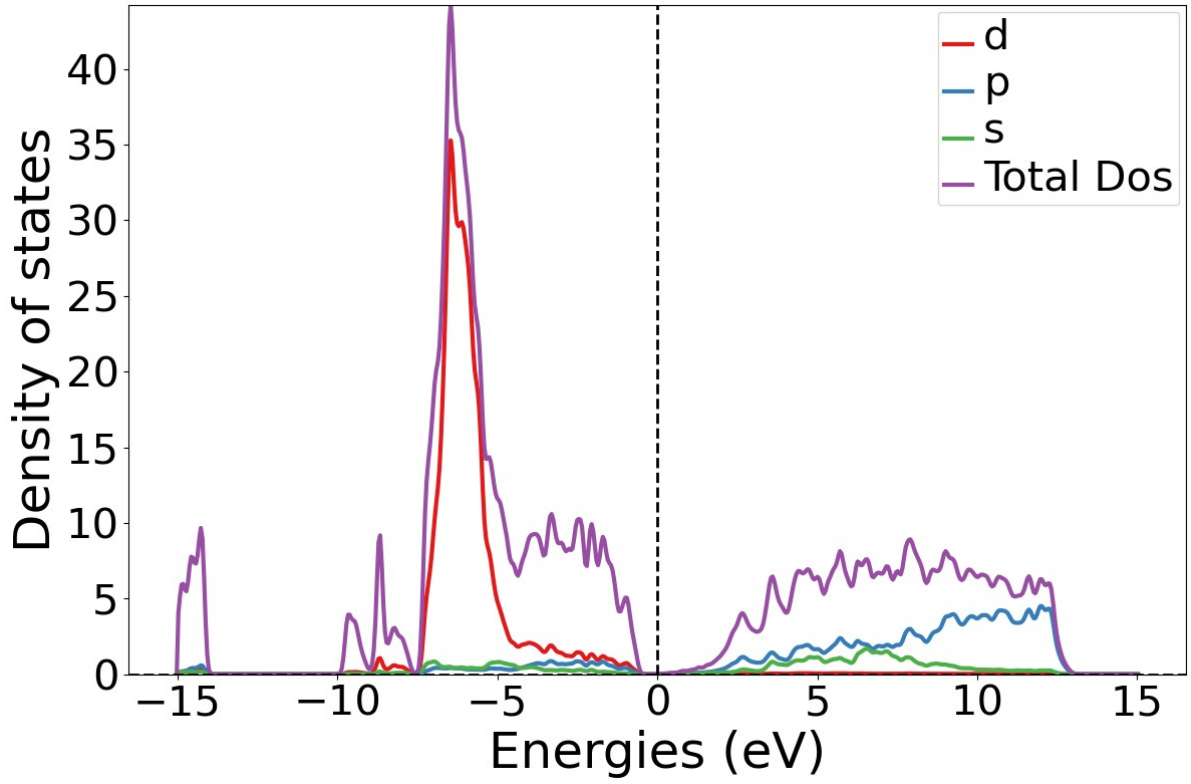

Figure S6: Orbital separated pDOS of the Zn orbitals

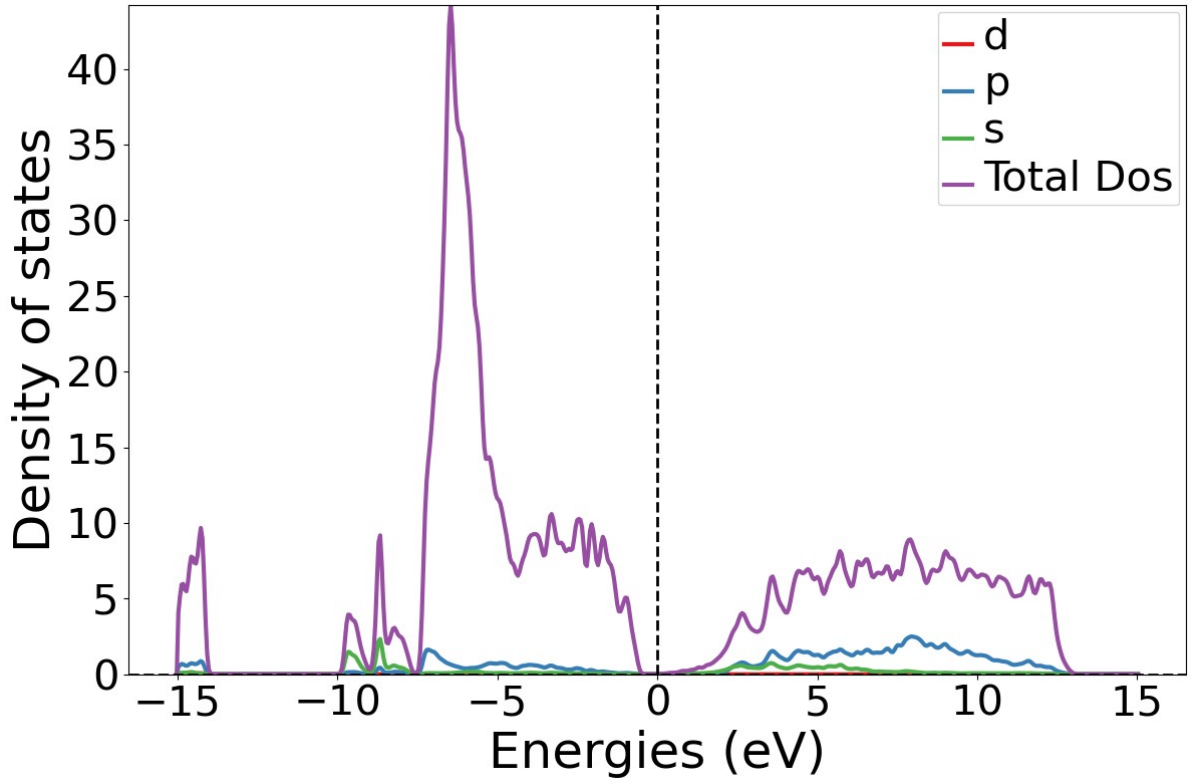

Figure S7: Orbital separated pDOS of the Ge orbitals

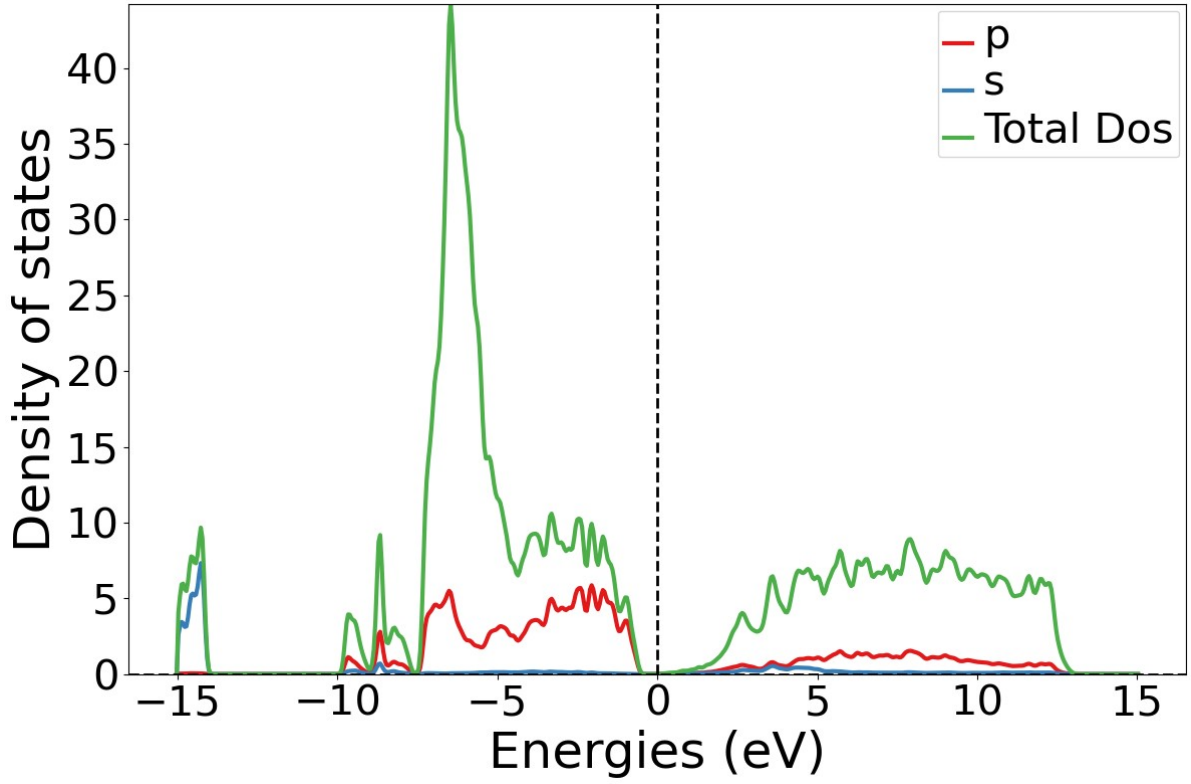

Figure S8: Orbital separated pDOS of the N orbitals

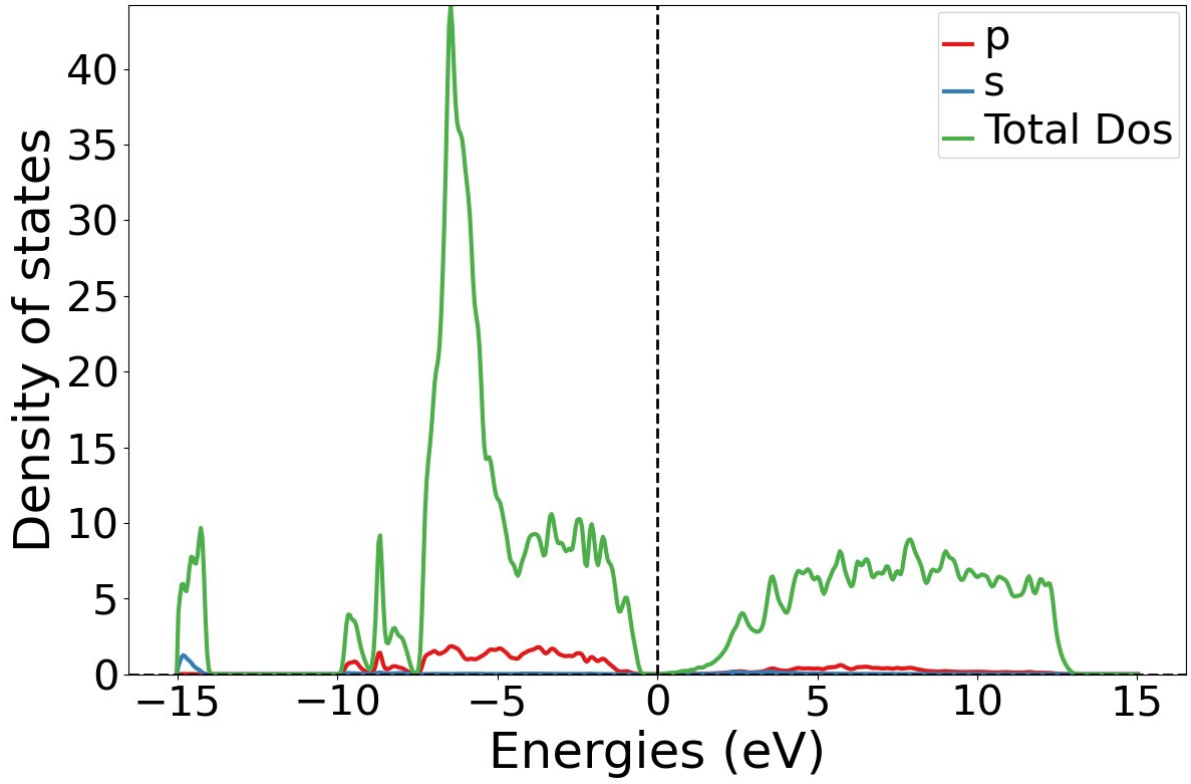

Figure S9: Orbital separated pDOS of the O orbitals

3. DOS of $Zn_{1.25}Ge_{0.75}(N_{0.75}O_{0.25})_2$ (b)

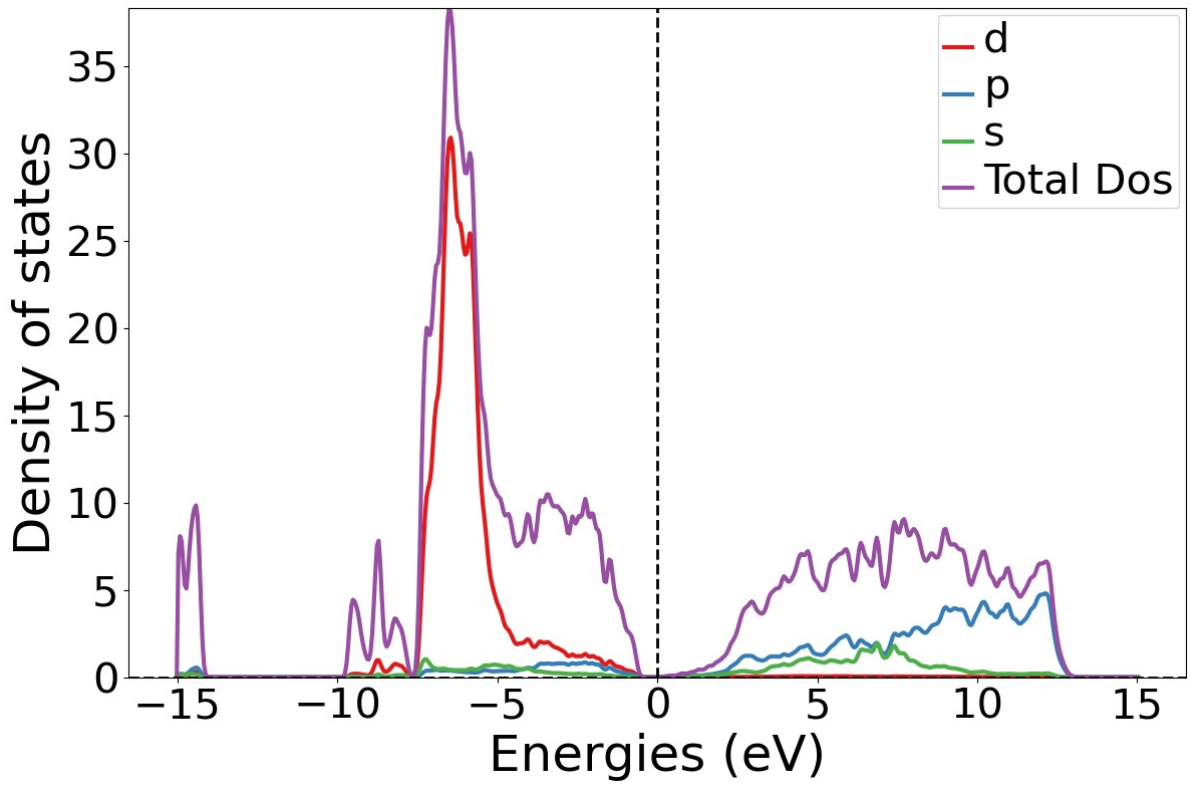

Figure S10: Orbital separated pDOS of the Zn orbitals

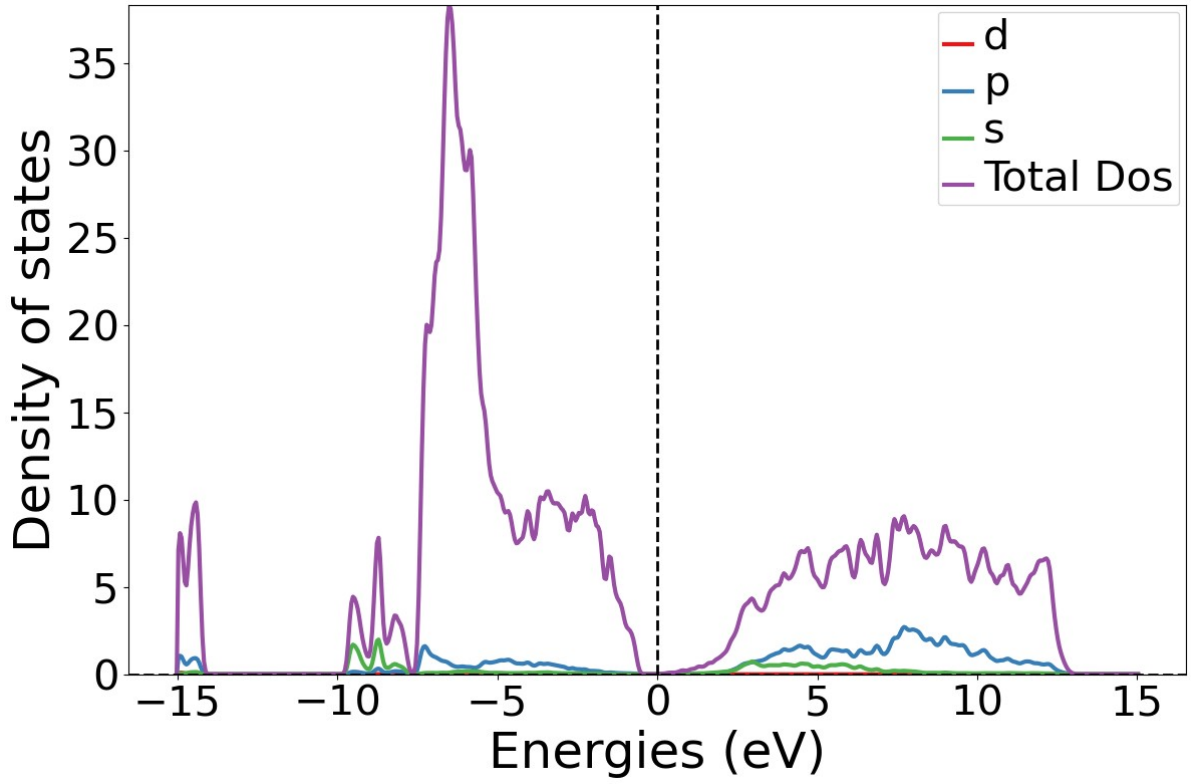

Figure S11: Orbital separated pDOS of the Ge orbitals

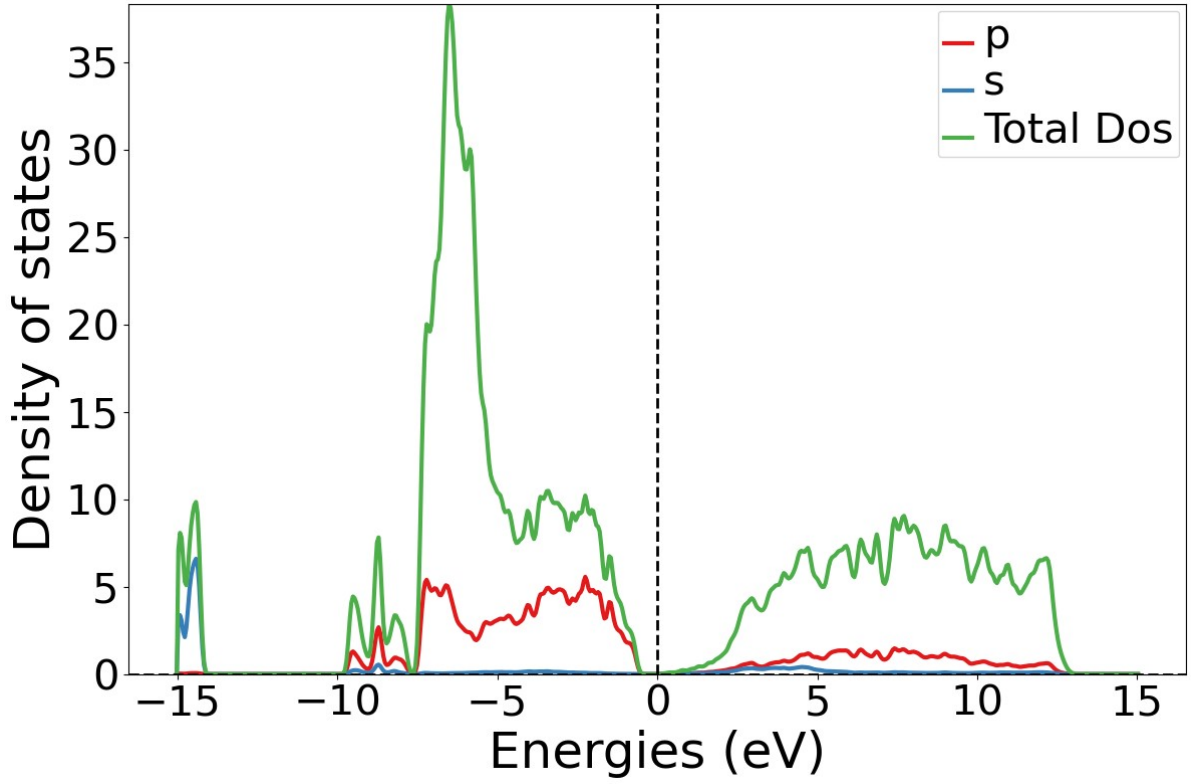

Figure S12: Orbital separated pDOS of the N orbitals

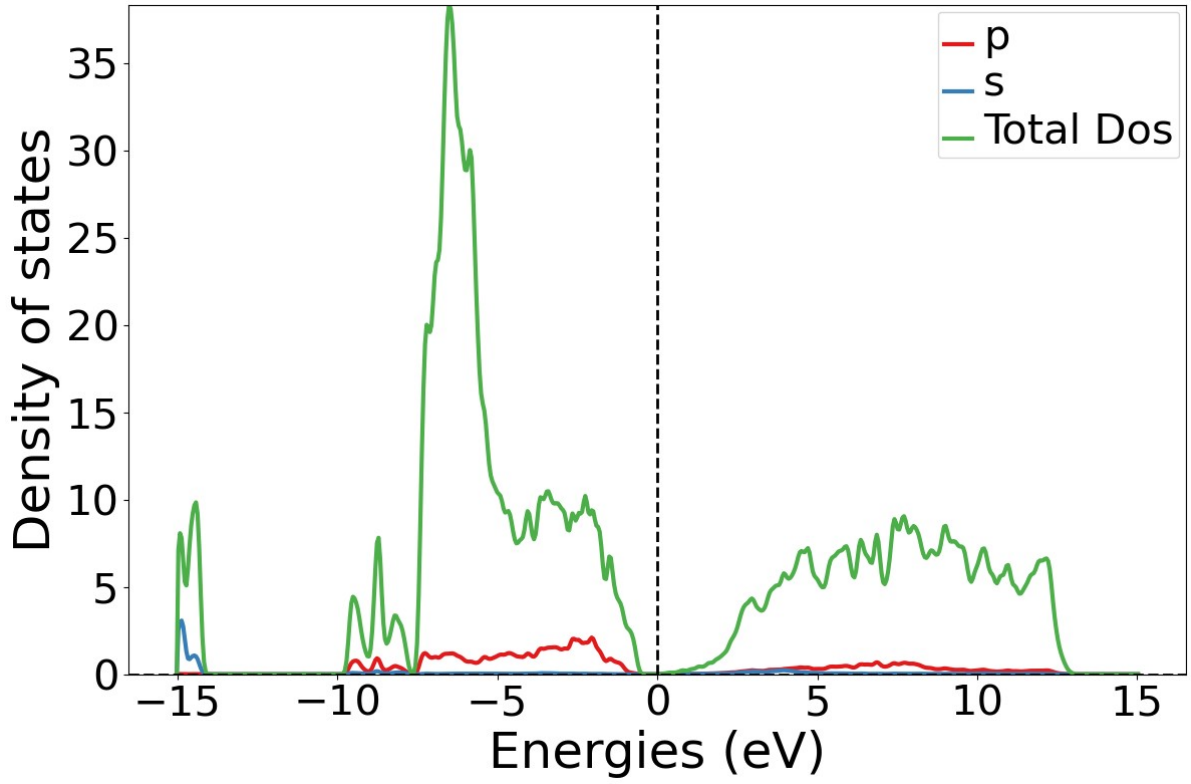

Figure S13: Orbital separated pDOS of the O orbitals

4. COHP of $Zn_{1.25}Ge_{0.75}(N_{0.75}O_{0.25})_2$ (a)

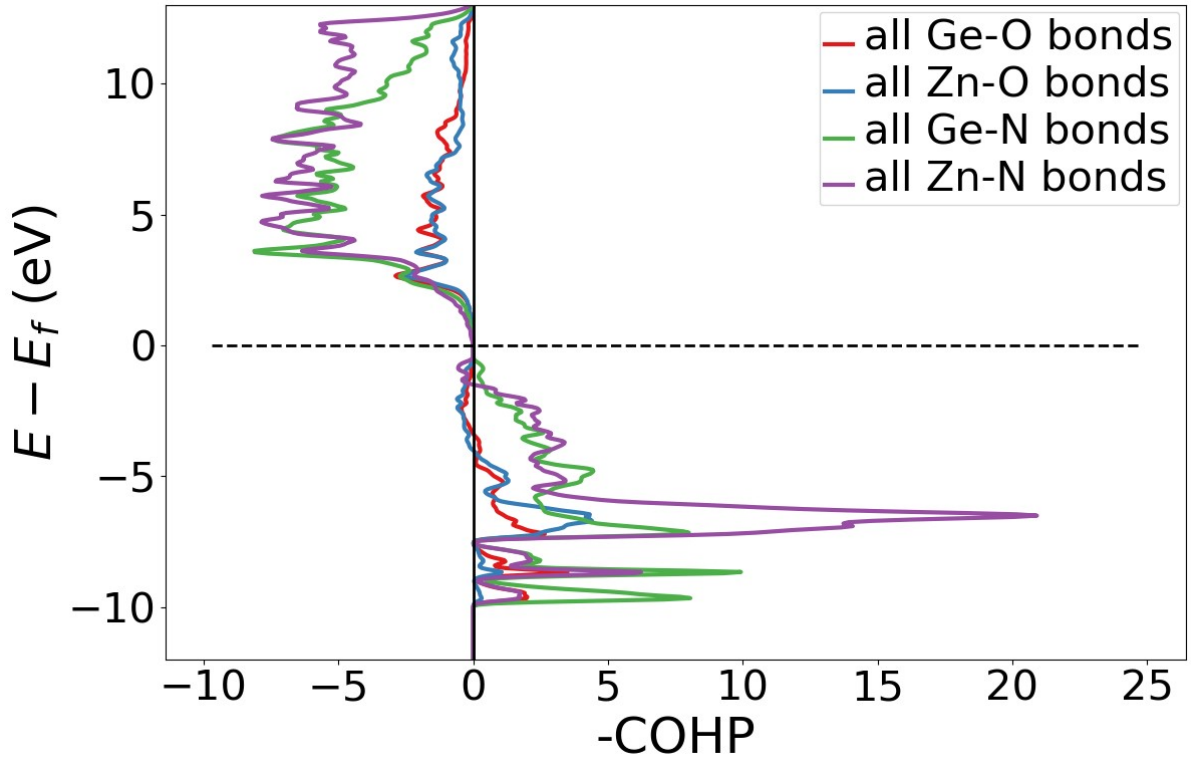

Figure S14: COHPs summed over the Ge-N, Zn-N, Ge-O and Zn-O bonds.