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Native point defects and doping in $ZnGeN_2$[1] DMITRY SKACHKOV, WALTER LAMBRECHT, Case Western Reserve University — A computational study within the framework of density functional theory is presented for native defects and doping in $ZnGeN_2$. We study the three types of vacancies V_{Zn}, V_{Ge}, V_N, cation antisite defects Zn_{Ge}, Ge_{Zn}, and potential n-type (O_N, Ga_{Zn}) and p-type Ga_{Ge} dopants. The cation antisite defects are found to have significantly lower formation energy than the cation vacancies. The charge neutrality condition pins the Fermi level close to the the crossing of the Zn_{Ge}^{-1} acceptor with the Ge_{Zn}^{2+} donor, and intrinsic p-type doping would result. The V_N is found to be a rather deep donor. Ge_{Zn} is found to behave as a shallow donor. Oxygen impurities are found to strongly prefer the O_N subsitutional site and are found to be shallow donors with a very low energy of formation. Energies of formation of Ga_{Zn} and Ga_{Ge} are lower than those of the cation antisites. Thus good solubility is expected and these impurities can hence pin the Fermi level at the crossing of the donor Ga_{Zn}^{+1} with the acceptor Ga_{Ge}^{-1}, and efficient p-type doping should result.

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