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Engineering Electronic and Magnetic Properties of $(A_xGa_{1-x})_2O_3$ [A=In or Tl] Alloys SHARAD MAHATARA, BORIS KIEFER, New Mexico State University — Bandgap engineering aims at creating and controlling electronic states that can support specific technological applications. An example of bandgap engineering is the doping of β-Ga_2O_3 (E_g∼4.8 eV), a wide gap insulator, that enables applications in UV sensing and in advanced power electronics. In this contribution, we use a Hubbard-U modified version of density-functional-theory (DFT) to study electronic effects of In and Tl dopants as well as vacancies on material properties of β-Ga_2O_3. We compare and contrast the electronic properties of little studied $(Tl_xGa_{1-x})_2O_3$ with those of the much better characterized $(In_xGa_{1-x})_2O_3$ alloys. Our calculations show that Tl-doping requires ∼4 times less doping to transverse the complete UV range as compared to In-doping, while showing comparable thermodynamic behavior. Spin-polarized calculations show that tetrahedral and octahedral Ga vacancies lead to spin-polarized ground states in both doped and undoped β-Ga_2O_3. Thus, $(Tl_xGa_{1-x})_2O_3$ may not only be of interest for optoelectronics but also as a materials platform for spintronics applications

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