Our new paper in Materials Research Express

Congratulations to our new paper “Structural Stability and Electron Density Analysis of Doped Germanene: A First-Principles Study” by
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The optimized geometry and electronic properties of doped germanene are studied by first-principles calculations. The band structure and density of states of germanene with dopants of group III (Al, Ga and In), IV (Si and Sn), and V (P, As and Sb) are investigated. The results show that group III dopants change the intrinsic behavior of germanene to p-type semiconductor, whereas group V dopants make germanene n-type semiconductor. Moreover, the pristine behavior of germanene remains unchanged by dopants of group IV. The stability of doped optimized supercells and the stability of dopants are obtained by different thermodynamic parameters such as cohesive, and relative binding energies. The binding energies are related to the localization of electrons and shown by electron localization function plots. The n-type, p-type, and intrinsic characteristics are studied by charge transfer calculation and electron difference density plots, to show how electron or hole is injected to the lattice. We found that how the stability features and the electronic properties of doped structures are related to the changes in electron density with doping. In addition, we study the charge transfer and stability of adatoms on germanene and dopants in bulk germanium. Adatoms have lower charge transfer than doped germanene, while dopants in bulk germanium have higher charge transfer values. Based on the calculated results of the

present work, the adatoms are more stable than the inserted dopants in germanene.