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Mechanical and electronic properties of pristine and Ni-doped Si, Ge, and Sn sheets AADITYA MANJANATH, Indian Institute of Science, Bangalore 560012 INDIA, VIJAY KUMAR, Dr. Vijay Kumar Foundation 969, Sector 4, Gurgaon 122 001, Haryana, India, ABHISHEK SINGH, Indian Institute of Science, Bangalore 560012 INDIA — Silicene, a graphene analogue of silicon, has been generating immense interest due to its potential for applications in miniaturized devices. Unlike planar graphene, silicene prefers a buckled structure. Here we explore the possibility of stabilizing a planar form of silicene by Ni doping using first principles density functional theory based calculations. It is found that planar as well as buckled structure is stable for the Ni doped silicene, but the buckled sheet has slightly lower total energy. The planar silicene sheet has unstable phonon modes. A comparative study of the mechanical properties reveals that the in-plane stiffness of both the pristine and the doped planar silicene is higher compared to that of the buckled silicene. This suggests that planar silicene is mechanically more robust. Electronic structure calculations of the planar and buckled Ni-doped silicene show that the energy bands at the Dirac point transform from linear behavior to parabolic dispersion. Furthermore, we extend our study to Ge and Sn sheets that are also stable and the trends of comparable mechanical stability of the planar and buckled phases remain the same.

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