Two- and one-dimensional honeycomb structures of silicon and germanium

SEYMUR CAHANGIROV, MEHMET TOPSAKAL, ETHEM AKTURK, HASAN ŞAHIN, SALIM CIRACI

1 UNAM - Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey, CIRACI GROUP TEAM — First-principles calculations of structure optimization, phonon modes and finite temperature molecular dynamics predict that silicon and germanium can have stable, two-dimensional, low-buckled, honeycomb structures. Similar to graphene, these puckered structures are ambipolar and their charge carriers can behave like a massless Dirac fermions due to their $\pi$- and $\pi^*$-bands which are crossed linearly at the Fermi level. In addition to these fundamental properties, bare and hydrogen passivated nanoribbons of Si and Ge show remarkable electronic and magnetic properties, which are size and orientation dependent. These properties offer interesting alternatives for the engineering of diverse nanodevices.

1Department of Physics, Bilkent University, Ankara

Seymur Cahangirov

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