

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Monolayer Honeycomb Structures of Group-IV Elements and III-V Binary Compounds: First-principles Calculations HASAN SAHIN, S. CAHANAGIROV, M. TOPSAKAL, E. BEKAROGLU, E. AKTURK, Bilkent University- UNAM, R. TUGRUL SENGER, IYTE-Izmir Institute of Technology, SALIM CIRACI, Bilkent University, UNAM-Institute of Materials Science and Nanotechnology — Using first-principles plane-wave calculations, we investigate two-dimensional (2D) honeycomb structure of group-IV elements and their binary compounds as well as the compounds of group III-V elements. Based on structure optimization and phonon-mode calculations, we determine that 22 different honeycomb materials are stable and correspond to local minima on the Born-Oppenheimer surface. We also find that all the binary compounds containing one of the first row elements, B, C, or N have planar stable structures. On the other hand, in the honeycomb structures of Si, Ge, and other binary compounds the alternating atoms of hexagons are buckled since the stability is maintained by puckering. For those honeycomb materials which were found stable, we calculated optimized structures, cohesive energies, phonon modes, electronic-band structures, effective cation and anion charges, and some elastic constants. The band gaps calculated within density functional theory using local density approximation are corrected by GW_0 method. Si and Ge in honeycomb structure are semimetal . . .

Hasan Sahin
Bilkent University, UNAM-Institute of Materials Science
and Nanotechnology

Date submitted: 03 Dec 2009

Electronic form version 1.4