First-principles study of group IV honeycomb layers and their binary alloys

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Graphene, a two dimensional system exhibits exceptional electronic and physical properties, which have led to the extremely extensive research activities and wide range of proposed applications in nano-electronics and other fields. However, it has been recently predicted theoretically that other group IV elements (Si, Ge, Sn) can be stabilized in the form of honeycomb two-dimensional lattices and soon such materials have been really synthetized [1] and silicene, germacene, and stanene have been born. Soon has been reported that the binary alloys of group IV elements (SiC, SiGe, etc.) can be also stabilized in a form of honeycomb monolayers [2]. Motivated by these developments we have undertaken extensive *ab initio* (in the frame work of the density functional theory) studies of cohesive and electronic properties of the whole plethora of the honeycomb monoatomic systems. We have employed the *VASP* numerical package [3] to compute phase diagrams and electronic band structures of the following systems: Si-Si (silicene), Ge-Ge (germacene), Sn-Sn (stanene) and the binary alloys Si-C, Ge-C, Sn-C, Si-Ge, Si-Sn, and Ge-Sn. For the phase diagram calculations, we consider so-called high buckled and low buckled structures as depicted in the Fig. 1.

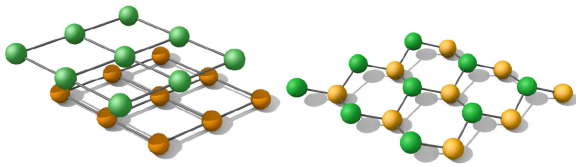

Figure 1 High and low buckled honeycomb lattices. In high buckled structure the vertical distance between atoms is typically larger than the lateral one.

The typical phase diagram of the binary alloys is presented for Si-Ge alloy in Fig. 2.

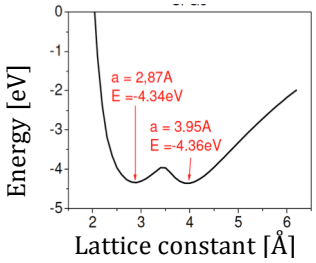

Figure 2 Phase diagram for the Si-Ge. The low buckled phase has the lower energy by 20 meV in comparison to the high buckled one. The equilibrium lattice constants of the low and high buckled phases are equal to 3.95 Å and 2.87 Å, respectively. The relatively small difference between energy minima of the two phases is characteristic for all binary alloys not containing carbon.

The alloys containing C, Si-C, Ge-C, and Sn-C, have nearly flat low buckled equilibrium phase and the equilibrium energy of this phase is considerably lower than of the high buckled phase. It is in contrary to all other alloys where the energetic differences are rather small (see Fig. 1). It strongly suggests that such structures could be transformed into each other under suitable stress. Si-C, Ge-C, and Sn-C alloys have also large energy gap (roughly 2 eV), whereas all other systems have zero or minimal energy gap.

[1] For a review see e.g., Pere Miro *et al*., *Chem. Soc. Rev.* **43**, 6537 (2014).
[2] E. Bekaroglu *et al*., *Phys. Rev. B* **81**, 075433 (2010); H. Zhou *et al*., *J. Phys.:Condens. Matter* **25**, 395501 (2013); D. Kaplan *et al*., *J. Appl. Phys*. **113**, 183701 (2013); P. Li et al. *Nanoscale*, Advance Article (2014).
[3] G. Kresse and J. Hafner, *Phys. Rev. B* **47**, 558 (1993).