Introduction to Silicene for Molecular Dynamics Simulations

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Silicene, a two-dimensional silicon monolayer possessing hexagonal honeycomb lattice with a buckled height of ~ 0.44 Å has recently afforded great appeal as a novel graphene-like material.

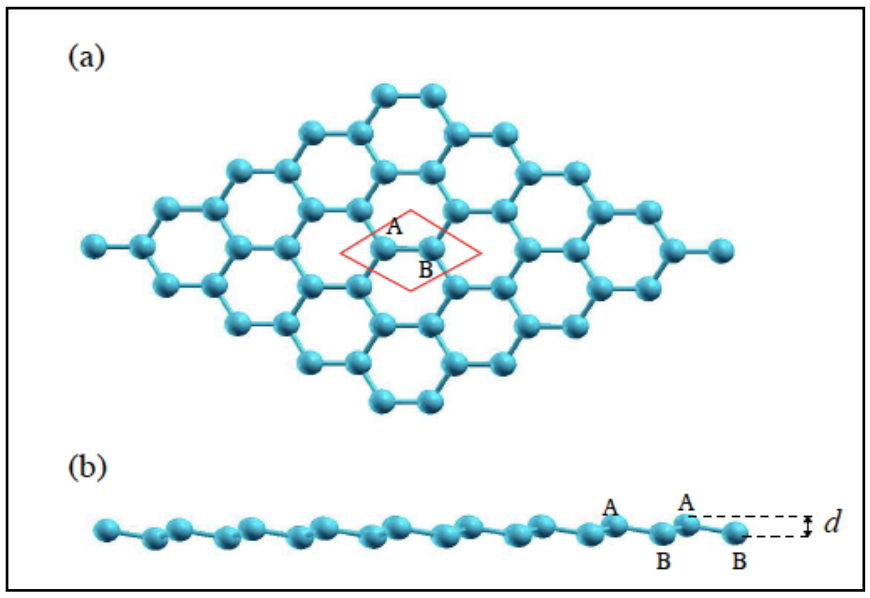


Fig.1 Top view (a) and side view (b) of silicene.
Bond length and bond angles are ~2.28 Å and 115.4° respectively. The value of bond angle lies in between those of sp^2 (120°) and sp^3 (109.47°) hybridized structures. This shows that hybridization in silicene is not purely sp^2 but a mixture of sp^2 and sp^3
Compared with graphene, the larger Si-Si interatomic distance weakens the π-π overlaps, so it cannot maintain the planar structure anymore.

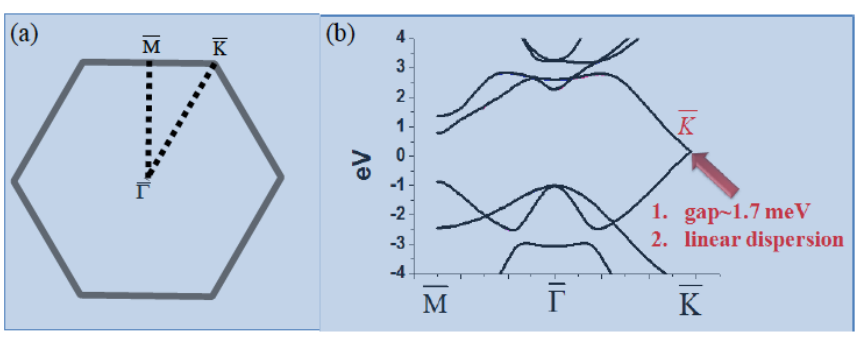
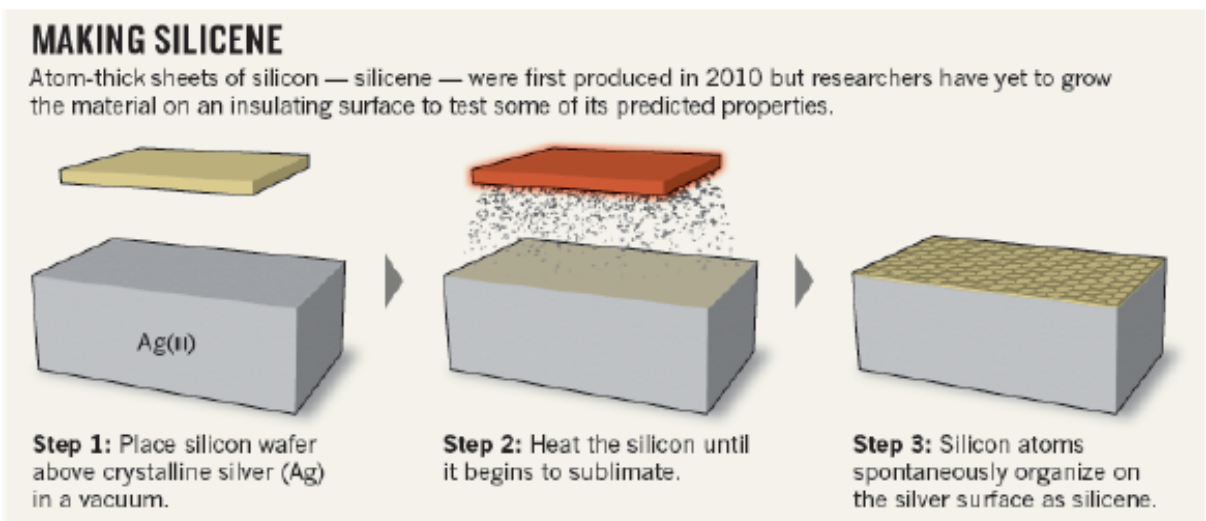


Fig.2 (a) Schematic of the first Brillouin Zone of silicene and its points of high symmetry.
(b) Band structure of silicene. Zero of energy set at the Fermi level. There is a small band gap at K and bands are linear near the cross section point K.

Very excitingly, silicene possess most of the astonishing electronic properties of graphene sheets:

- Charge carriers predicted to be massless Dirac Fermions due to the linear dispersion around the Fermi level at the symmetric point K in the reciprocal lattice [1].
- The spin-orbit coupling is even stronger in silicene, with regard to graphene, resulting in a more significant quantum spin Hall effect [2].
- First-principle calculations predict a tunable gap can be opened up at the Fermi level via functionalization or applying electric Field [3-5].
- Most attractively, the easier integration into current Si-based technology makes silicene a potential candidate for microelectronic devices.

Until now, free-standing silicene has never been observed.
Much efforts have been devoted to grow silicene on substrates
First synthesis on Ag (111) in 2010 by CVD [6]



- Ultra High Vacuum conditions
- Substrate temperature kept between 220 and 250 °C
- Rate of deposition of silicon lower than 0.1 monolayer per minute.
- **Variety of superstructures were observed depending on temperature and deposition rate.**

- **There are still many unanswered questions about the growth mechanism of silicene on substrates.**
- **Theoretical modeling of structures (using molecular dynamics) is not yet at the level of predicting the superstructures.**
- **Another, yet unanswered question, is the possibility to synthesize silicene sheets using Plasma Enhanced Chemical Vapor Deposition technique.**

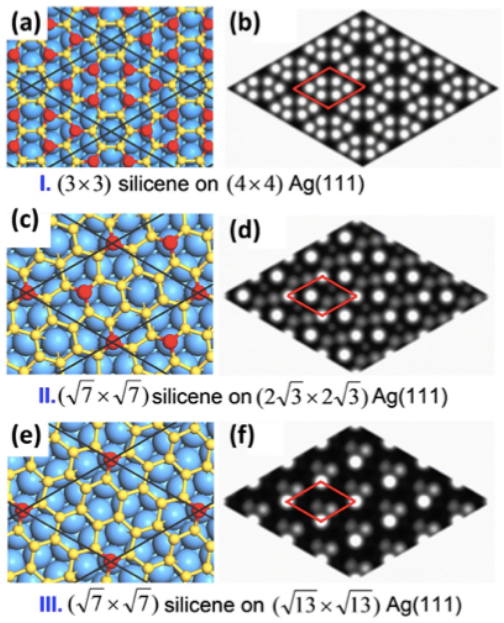


Fig.3 (a),(c),(e) Atomic structures of three types of silicene on Ag(111) superstructures and (b),(d),(f) their corresponding STM images [7].

Currently, the energies and temperature dependent dynamics of free-standing silicene are performed using Density functional theory and molecular dynamics (MD) simulations (ab initio and classical) to understand the structural properties and thermal stabilities
VASP [8] and LAMMPS [9] codes are used for ab intio and classical MD calculations respectively.

[1] Phys. Rev. Lett. 2012, 108 (15), 155501
[2] Phys. Rev. Lett. 2011, 107 (7), 076802
[3] Chem. Phys. Lett. 2011, 511 (1–3), 101
[4] Appl. Phys. Lett. 2012, 100 (8), 083102
[5] Phys. Rev. B 2012, 85 (7), 075423
[6] Appl. Phys. Lett. 2010, 97 (22), 223109
[7] Surface. Sci. Rep. 2012, 2, 861
[8] Comput. Mat. Sci. 1996, 6,15
[9] J Comp Phys. 1995 117, 1-19