

Engineering Silicene by Defects

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ABSTRACT

Recent experimental progress has made synthesis of monolayer silicon, silicene, possible. Our studies have revealed that unlike graphene, silicene has highly reactive crystal structure and formation of Stone-Wales type defects is more likely.

ADATOMS

The adsorption characteristics of alkali, alkaline-earth, and transition metal adatoms on silicene, a graphene-like monolayer structure of silicon are analyzed by means of first-principles calculations [1-2]. In contrast to graphene, interaction between the metal atoms and the silicene surface is quite strong due to its highly reactive buckled hexagonal structure. Alkali metals, Li, Na, and K, adsorb to hollow sites without any lattice distortion. As a consequence of the significant charge transfer from alkalis to silicene, metallization of silicene takes place. We found that the adsorption of alkaline-earth metals on silicene is entirely different from their adsorption on graphene. The adsorption of Be, Mg, and Ca turns silicene into a narrow gap semiconductor. Adsorption characteristics of eight transition metals Ti, V, Cr, Mn, Fe, Co, Mo, and W are also investigated. As a result of their partially occupied d orbital, transition metals show diverse structural, electronic, and magnetic properties. Upon the adsorption of transition metals, depending on the adatom type and atomic radius, the system can exhibit metal, half-metal, and semiconducting behavior. For all metal adsorbates, the direction of the charge transfer is from adsorbate to silicene, because of its high surface reactivity. Our results indicate that the reactive crystal structure of silicene provides a rich playground for functionalization at nanoscale.

STONE-WALES DEFECTS

During the synthesis of ultrathin materials with hexagonal lattice structure Stone-Wales (SW) type of defects are quite likely to be formed and the existence of such topological defects in the graphenelike structures results in dramatic changes of their electronic and mechanical properties. In our second study [2] investigate the formation and reactivity of such SW defects in silicene. We report the energy barrier for the formation of SW defects in freestanding (~ 2.4 eV) and Ag(111)-supported (~ 2.8 eV) silicene and found it to be significantly lower than in graphene (~ 9.2 eV). Moreover, the buckled nature of silicene provides a large energy barrier for the healing of the SW defect and therefore defective silicene is stable even at high temperatures. Silicene with SW defects is semiconducting with a direct band gap of 0.02 eV and this value depends on the concentration of defects. Furthermore, nitrogen substitution in SW-defected silicene shows that the defect lattice sites are the least preferable substitution locations for the N atoms. Our findings show the easy formation of SW defects in silicene and also provide a guideline for band gap engineering in silicene-based materials through such defects.

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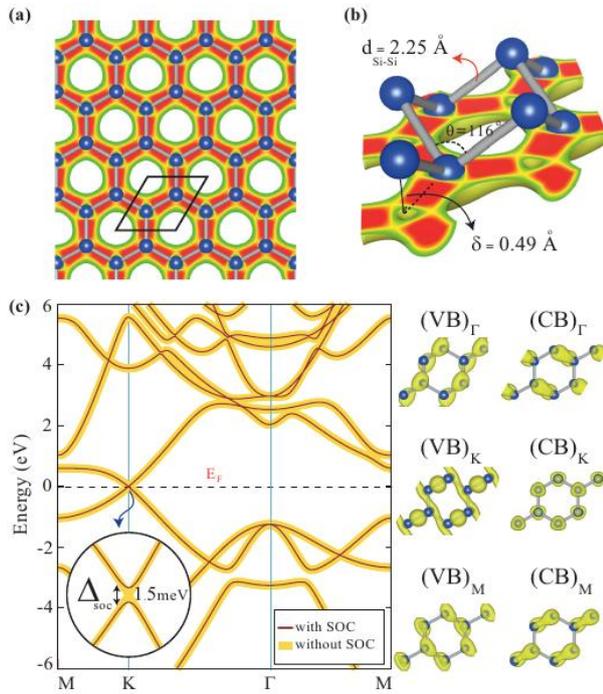


Fig. 1. Atomic and electronic structure of single layer silicene

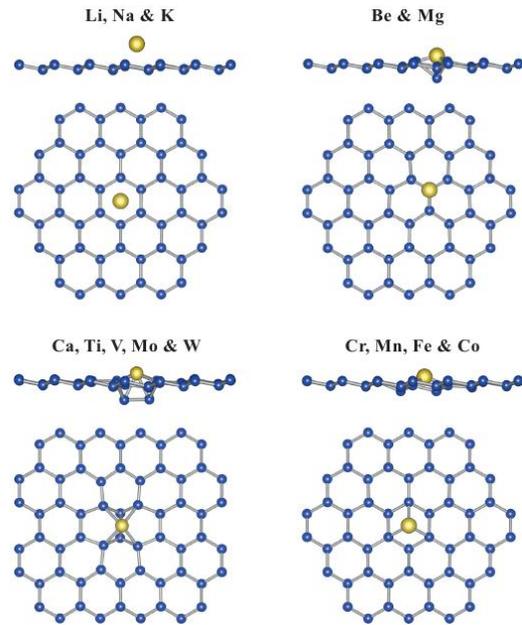


Fig. 2. Favorable adsorption sites for various metal adatoms

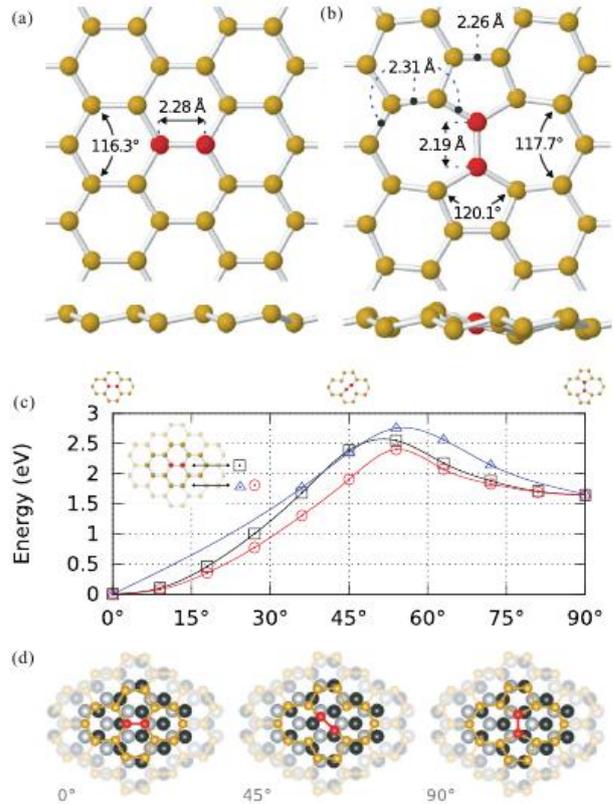


Fig. 3. Stone-Wales defects in single layer silicene