Ab initio Calculation of the Effect of Boron Doping on the Mechanical Properties of Silicene

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In this paper, we used density functional theory and pseudopotential calculations to investigate the structural and mechanical properties of boron-doped silicene. The total energy of atomic systems was calculated using the Quantum ESPRESSO code, using high-performance computing. PBE pseudopotentials for silicon and boron atoms, in the generalized-gradient approximation (GGA) were taken from the Quantum ESPRESSO code. We showed the substitution of silicon atoms by boron in silicene leads to its strong structural distortion. Furthermore, we found that Young's modulus for boron-doped silicene decreased.