Electron-Energy-Loss Spectra of Free-Standing Silicene 1

LUIS M. PRIEDE, CIDS-IC BUAP, LILIA MEZA-MONTES, Instituto de Física BUAP, E. GOMEZ-BAROJAS, CIDS-IC BUAP — Silicene, the silicon-based counterpart of graphene, is increasingly getting attention because it is a semi-metal material with Dirac cones and thus, in principle, has similar electronic properties [1, 2]. In this work we calculated the Electron Energy Loss Spectrum (EELS) of ideal free-standing silicene. Dielectric function is obtained by using a discretization method as suggested by Delerue, et al. [3]. Tight-binding method is applied considering 2nd Nearest Neighbors with $sp^2$ orbitals, the Slater-Koster parameterization [4] and the Harrison’s rule. This has been done for plane and buckled silicon sheets, in the latter case with a structure based on DFT calculations [2]. The resulting dielectric function is compared to those of bulk silicon and graphene. Spectra of EEELS are contrasted for plane and buckled silicene, particularly the plasmon frequency as a function of the $z$ displacement of buckled silicene.


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