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Unveiling the origin of the linear dispersion in silicene/Ag(111) MINGXING CHEN, MICHAEL WEINERT, Univ of Wisconsin, Milwaukee — The band structure of the recently synthesized (3×3) silicene monolayer on (4×4) Ag(111) is investigated using density functional theory. To compare to recent angleresolved photoemission spectroscopy (ARPES) experiments [Phys. Rev. Lett. 108, 155501 (2012)], including the photon energy (k_{\perp}) dependence of the spectra, we use a k-projection technique to unfold the supercell bands of both silicene and the substrate onto the corresponding primitive cells. Our calculations reproduce the observed linear dispersion across the K point of (1×1) silicene observed, but demonstrate that this is not a Dirac state, but rather originates from the Ag(111) substrate, thus resolving the controversy concerning the origin of the linear dispersion in silicene/Ag(111).

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