Unveiling the origin of the linear dispersion in silicene/Ag(111)
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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 angle-
resolved 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 demon-
strate 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 sil-
icene/Ag(111).