

Efficient n -type Doping in Epitaxial Graphene through Strong Lateral Orbital Hybridization of Ti Adsorbate

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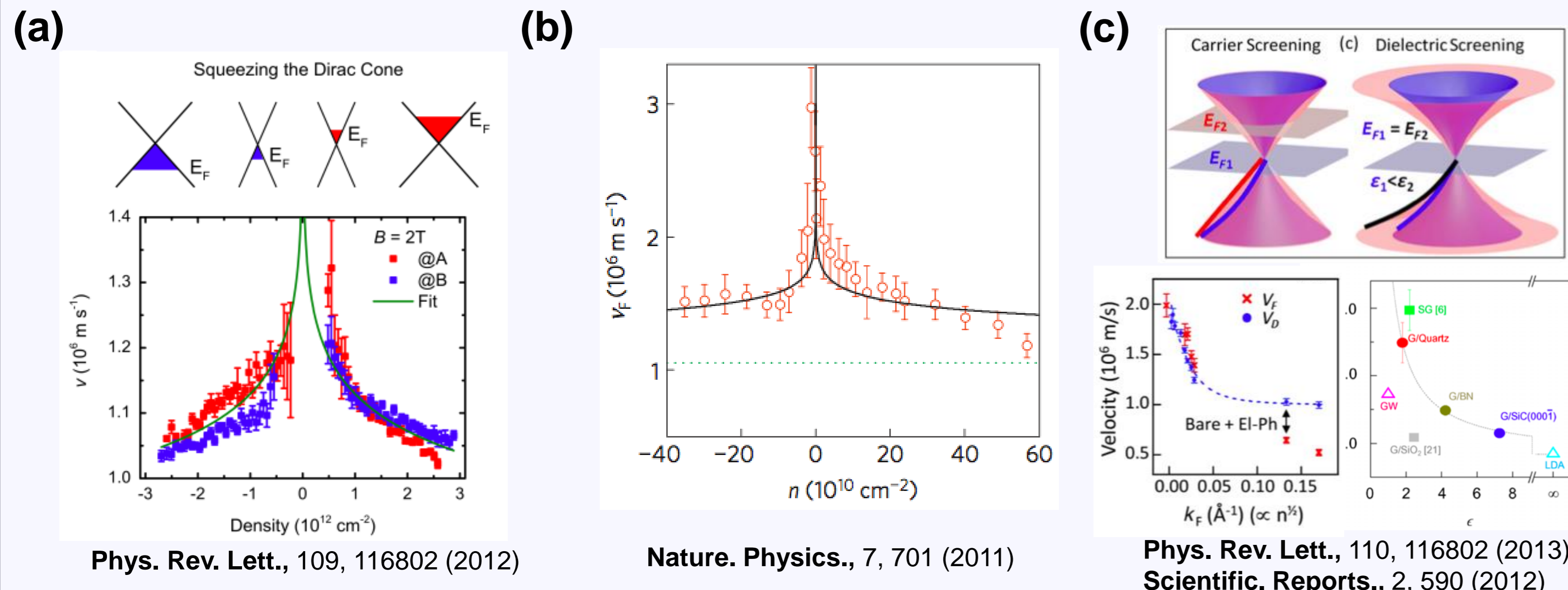
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ABSTRACT

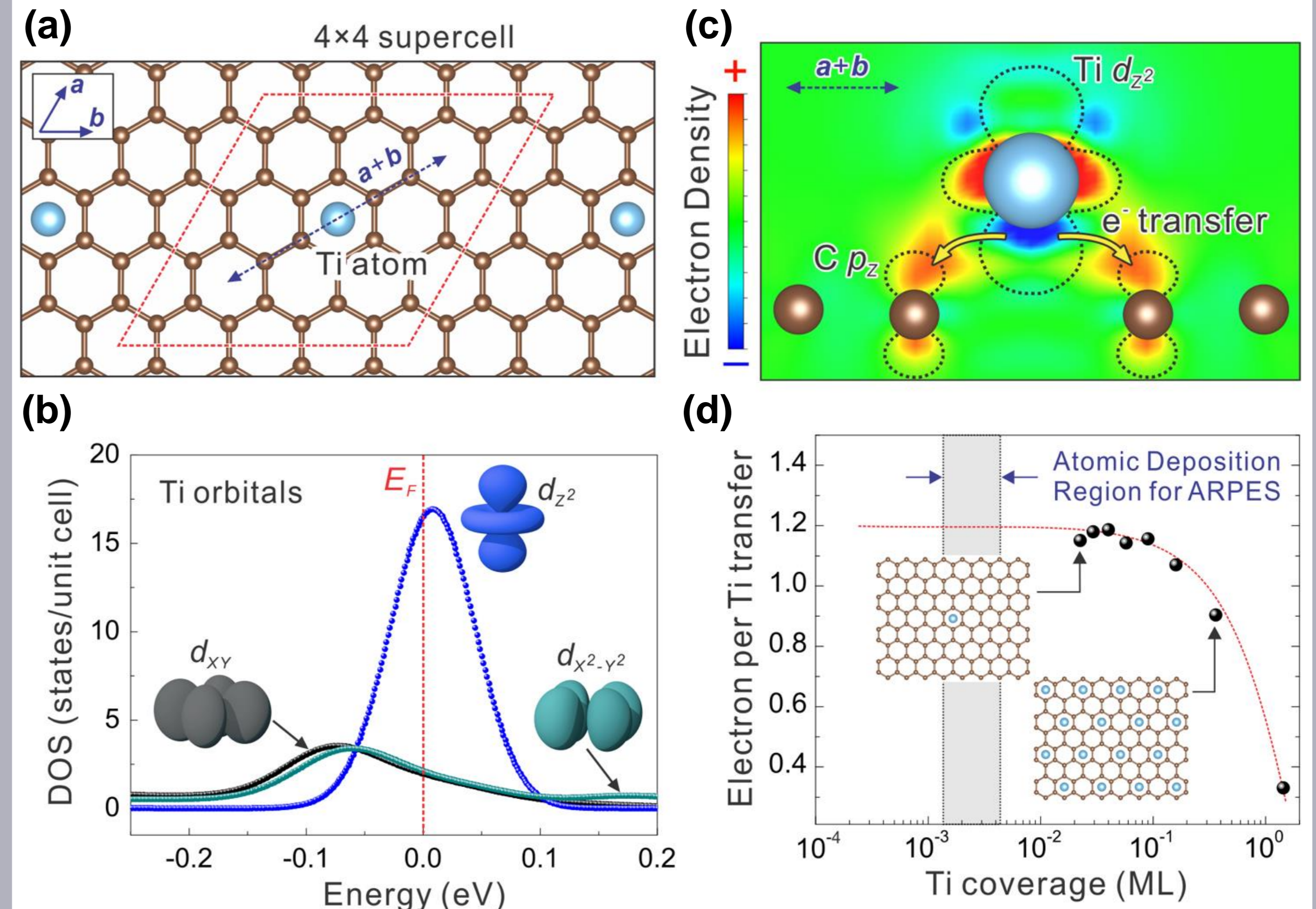
Recently, many different types of doping methods for epitaxial graphene have been demonstrated through atom substitution and adsorption. Then, here we observe by angle-resolved photoemission spectroscopy (ARPES) a coupling-induced Dirac cone renormalization when depositing small amounts of Ti onto epitaxial graphene on SiC. We obtain a remarkably high doping efficiency and a readily tunable carrier velocity simply by changing the amount of deposited Ti. First-principles theoretical calculations show that a strong lateral (non-vertical) orbital coupling leads to an efficient doping of graphene by hybridizing the $2p_z$ orbital of graphene and the $3d$ orbitals of the Ti adsorbate, which attached on graphene without creating any trap/scattering states. This Ti-induced hybridization is adsorbate-specific and has major consequences for efficient doping as well as applications towards adsorbate-induced modification of carrier transport in graphene.

Keywords - Graphene, lateral coupling, titanium, angle-resolved photoemission spectroscopy (ARPES), density-functional theory (DFT)

Introduction



First-Principle calculation



Angle-Resolved Photoemission Spectroscopy

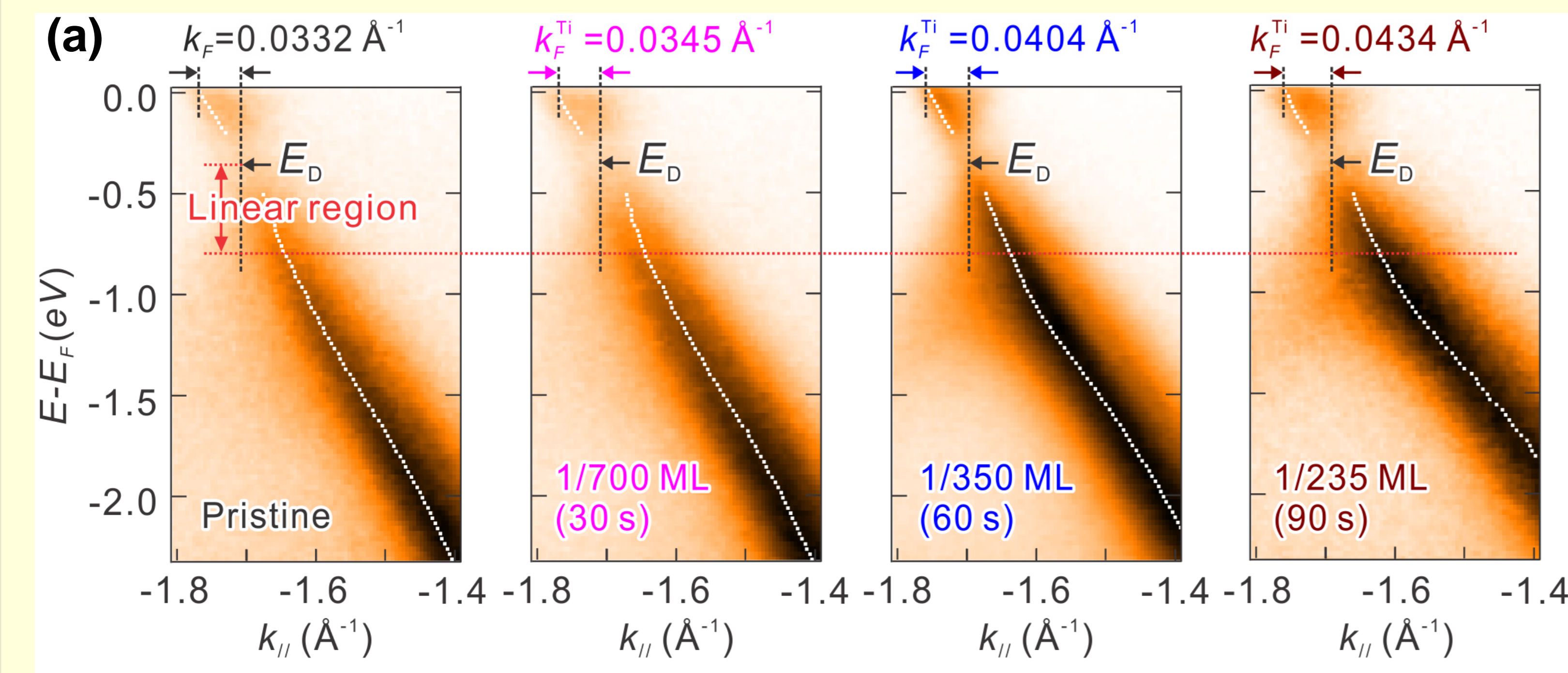


Fig 2. The ARPES measurements on graphene with Ti adatoms using an incoming SR photon energy of 52 eV at room temperature.

(a) \rightarrow Band structure of Ti-doped graphene for 0, 1/700, 1/350, and 1/235 ML coverage, taken along the $\mathbf{K} \rightarrow \Gamma$ direction and in the vicinity of the K-point. The energy dispersion is fitted by the MDCs (white dashed lines). The black arrow marks the binding energy position of the Dirac point. The acquired Fermi momentum k_F values are given.

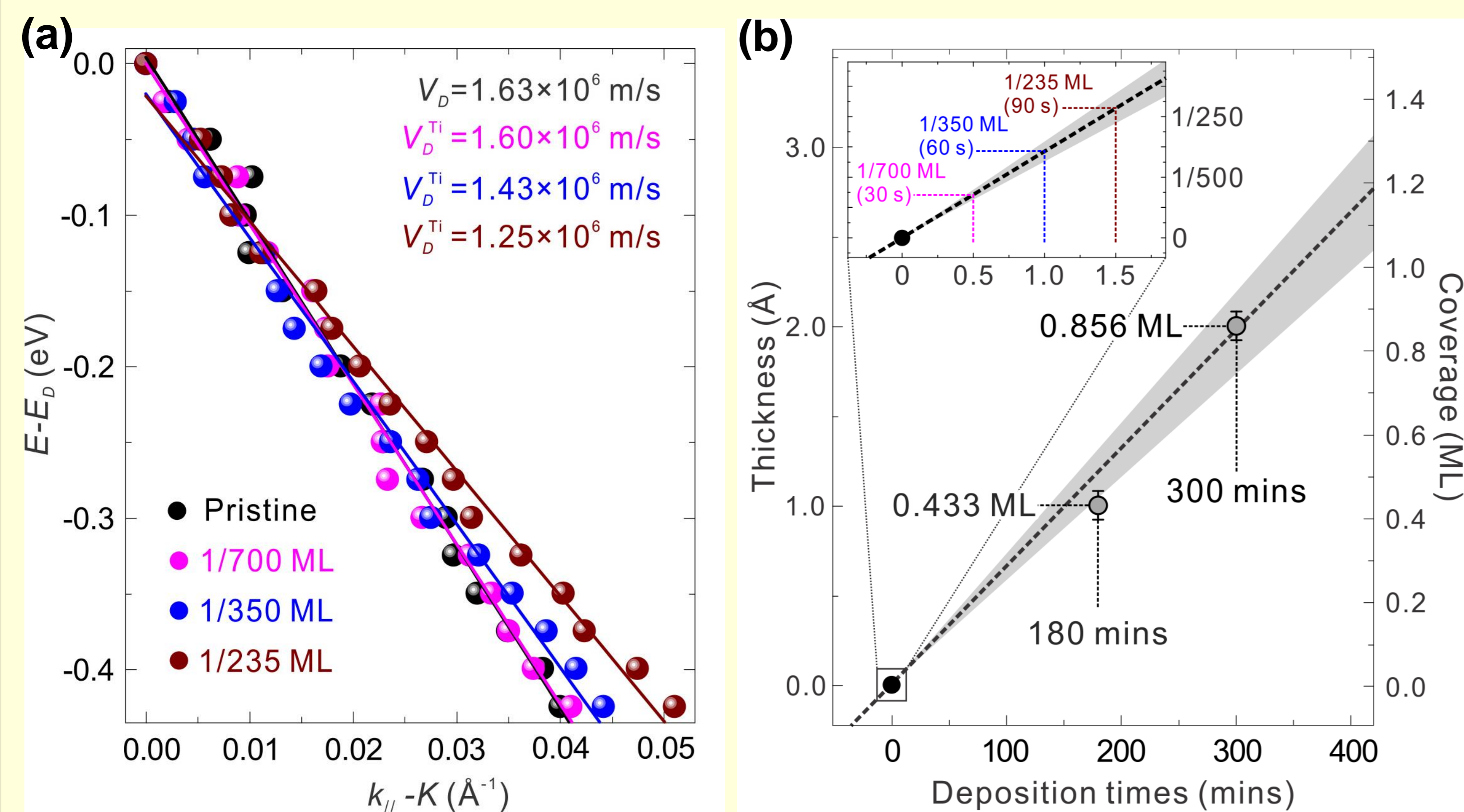


Fig 3. Band dispersion and Ti adatom coverage estimation

(a) \rightarrow Dirac velocity in the low-lying valence band depends on Ti coverage.
 (b) \rightarrow The Ti coverage calibration obtained by QCM. Deposition conditions and corresponding Ti coverages are listed. The black dashed line shows a least squares fit to the data.

Many-Body interaction

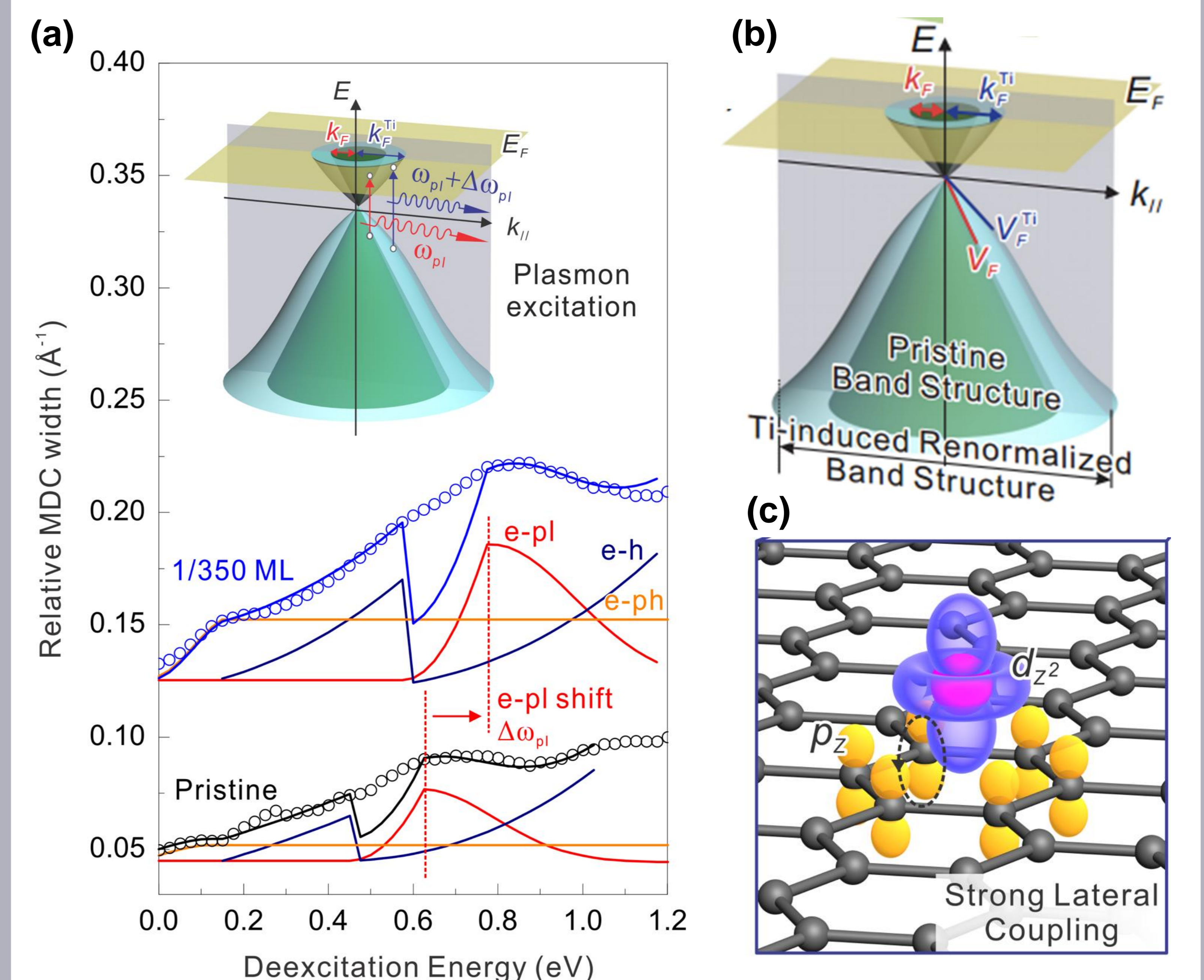


Fig 5. MDCs linewidths used to extract the many-body interaction on pristine and 1/350 ML doped epitaxial graphene.

(a) \rightarrow MDCs line-shape analysis is carried out by electron-phonon, electron-hole and electron-plasmon interaction.

(b) \rightarrow The electron-plasmon peak shift is associated to the renormalized electronic structures shown in the insert.

(c) \rightarrow Ti-3d and C-2p_z orbital hybridization.

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