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***Ab initio* study on atomic and electronic structures of epitaxial graphene** SEUNGCHUL KIM, JISOON IHM, Department of Physics and Astronomy, Seoul National University, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, YOUNG-WOO SON, Department of Physics, Konkuk University — Recently, lots of efforts have been devoted to the growth of epitaxial graphene and its geometric and electronic structure measurements. Several models for the interface structure have been suggested but never been successful in explaining the observations from various experiments. Using density functional theory (DFT) calculations, we find an interface atomic structure of graphene on hexagonal silicon carbide which agrees well with the low energy electron diffraction (LEED), scanning tunneling microscopy (STM), as well as angle resolved photo emission spectroscopy (ARPES). Our results clearly resolve the disagreement between 6×6 periodic pattern from STM measurements and the $6\sqrt{3} \times 6\sqrt{3}$ from the LEED measurements. Furthermore, we also investigate the origin of the gap opening at the Dirac point in the present geometry.

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