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Kekule-induced band-gap opening in graphene in contact with ZrO2 JUNG SUK GOH, HYOUNG JOON CHOI, Department of physics and IPAP, Yonsei University, Seoul 120-749, Korea — We have studied pressure-dependent atomic and electronic structure of graphene in contact with (111) surface of zirconium dioxide (ZrO2) using first-principles calculations. The atomic structures are optimized by relaxation, and we found that the lowest-energy configuration shows a band gap at the Dirac point at ambient pressure and the band gap increases as pressure increases. Our analysis shows that the band-gap opening is due to overlap of wavefunctions, change in potential energy, and in-plane distortion of graphene lattice. This in-plane distortion of graphene is found to be the Kekule distortion, which generates intervalley coupling. As pressure increases, the Kekule distortion in graphene increases and the band gap at the Dirac point is proportional to the size of the distortion. This work was supported by the NRF of Korea (Grant No. 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2012-C2-14).

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