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Ab initio scanning tunneling spectroscopy simulation of graphene with metal adatoms: weak and strong coupling regimes[1] GUNN KIM, Department of Physics, Kyung Hee University, Korea, JAE-HYEON PARQ, JAE-JUN YU, Department of Physics & Astronomy, Seoul National University, Korea, YOUNG-KYUN KWON, Department of Physics, Kyung Hee University, KYUNG HEE UNIVERSITY COLLABORATION, SEOUL NATIONAL UNIVERSITY COLLABORATION — Metal atoms on graphene, when ionized, can act as a point-charge impurity to probe a charge response of graphene with the Dirac cone band structure. To understand charge and spin polarization in graphene, we present scanning tunneling spectroscopy STS simulations based on density-functional theory calculations. We find that a Cs atom on graphene is fully ionized with a significant band-bending feature in the STS whereas the charge and magnetic states of Ba and La atoms on graphene appear to be complicated due to orbital hybridization and Coulomb interaction. By applying external electric field, we observe changes in charge donations and spin magnetic moments of the metal adsorbates on graphene.

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