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Incorporating isolated molybdenum (Mo) atoms into Bilayer Epitaxial Graphene on 4H-SiC(0001)[1] HAN HUANG, WEN WAN, Central South University, HUI LI, Institute of Physics, Chinese Academy of Sciences, SWEE LIANG WONG, National University of Singapore, LU LV, YONGLI GAO, Central South University, ANDREW T.S. WEE, National University of Singapore — The atomic structures and electronic properties of isolated Mo atoms in bilayer epitaxial graphene (BLEG) on 4H-SiC(0001) are investigated by low temperature scanning tunneling microscopy (LT-STM). LT-STM results reveal that isolated Mo dopants prefer to substitute C atoms at α-sites, and preferentially locate between the graphene bilayers. First-principles calculations confirm that the embedding of single Mo dopants within BLEG is energetically favorable as compared to monolayer graphene. The calculated bandstructures show that Mo-doped BLEG is n-doped, and each Mo atom introduces a local magnetic moment of 1.81 μ_B. Our findings demonstrate a simple and stable method to incorporate single transition metal dopants into the graphene lattice to tune its electronic and magnetic properties for possible use in graphene spin devices.

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