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Fluorinated graphene as an efficient diffusion barrier in Ge semiconductor devices WEI REN, HENG GAO, Shanghai University — We evaluate the efficient diffusion barrier effects of the fluorinated graphene from the first principles. By taking its advantage of impermeability, we discover such monoatomic layer can suppress the formation of the unstable interfacial oxide in Ge-based semiconductor devices. To elucidate the physical mechanism governing this shielding functionality, nudged elastic band method is adopted to calculate the barrier height of one oxygen or one germanium atom penetrating the pristine graphene and fluorinated graphene. The energy of the adsorbed O or Ge atom on different sites of the graphene is calculated, namely three positions on the honeycomb lattice, bridge, hollow, and top. Our results reveal that both the O and Ge atoms adsorbed on the graphene are most stable on the bridge site, followed by the top and hollow sites with higher energies. Different penetration paths of O and Ge atoms are considered, and the calculated values of the energy barriers for both graphene and fluorinated graphene exhibit superior impermeability and hence to hinder diffusion of O and Ge atoms across the graphene and fluorinated graphene. This latter insulating structure is expected to expedite the implementation of germanium as channel materials in next-generation nanoelectronic devices.

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