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Tuning Fe nucleation morphology via charge doping of graphene substrate[1] WENMEI MING, FENG LIU, Univ of Utah — Graphene with Fe deposition can be potentially used as magnetic storage device when Fe atoms assume island morphology, or as magnetic electric contact for spin injection in spintronics device when Fe atoms assume a uniform thin-film morphology. We propose that the Fe initial growth morphology on graphene can be tuned in a controllable manner via charge doping of graphene. On one hand, charge doping may either increase or decrease the bonding strength between Fe adatom and graphene, affecting Fe adsorption; on the other hand, it may modulate the Fe adatom–adatom interaction, affecting the Fe island nucleation. Using first principles calculations, we have investigated the following diverse effects of charge doping on Fe deposition on graphene as a function of doping concentration: (1) adatom adsorption energy; (2) local magnetic moment; (3) dipole moment; (4) elastic deformation energy; (5) adatom diffusion barrier; (6) adatom-adatom interaction. Furthermore, using kinetic Monte Carlo simulations augmented with first-principles parameters, we have studied the nucleation morphology of Fe deposition on the charge doped graphene. Our results shed new light on understanding and control of the growth morphology of metal atoms on graphene.

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