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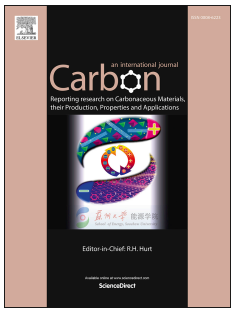

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Transition Metal Adatoms on Graphene: A Systematic Density Functional Study

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Abstract

Transition Metal (*TM*) atom adsorption on graphene results in a tuning of their electronic, magnetic, storage, sensing, and catalytic properties. Herein we provide a thorough density functional theory study, including dispersion, of the structural, energetic, diffusivity, magnetic, and doping properties for *all* 3*d*, 4*d*, and 5*d* TM adatoms adsorbed on graphene. TMs prefer to sit on hollow sites when chemisorbed, but on bridge or top sites when physisorbed; which is the case of atoms with d^5 and d^{10} configurations. Diffusion energy barriers follow the adsorption energy trends. Dispersive forces simply increase the adsorption strength by ~0.35 eV. Adatom height seems to be governed by the bond strength. All TMs are found to *n*-dope graphene, except Au, which *p*-dopes. The electron transfer decays along the *d* series due to the electronegativity increase. Early TMs infer noticeable magnetism to graphene, yet for elements with more than five electrons in the *d* shell the local magnetic moments abruptly decay to low or zero values. Experimental observations on adatom position, height, temperature clustering and Ostwald ripening, *p*- or *n*-doping, or the electronic configuration can be rationalized by present calculations, which deliver a solid theoretical ground from which experimental features can be interpreted and discussed.

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