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First-principles study of graphane with 3d transition-metal adatoms

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Recently, it has been established that the electronic properties of a graphane (hydrogenated graphene) sheet can be well tuned by foreign atom substitutions. This suggests that incorporating magnetic elements into its semiconducting environment could make graphane a good base for creating low dimensional dilute magnetic semiconductors for spintronic devices desirable for information storage and processing. Using DFT including the GGA + Hubbard U correction, we investigate the effects on structural, electronic and magnetic properties of graphane upon incorporation of 3d transition metal (Cr, Mn and Fe) adatoms on different adsorption sites. It is found that the high-spin configurations are more favourable for all the considered systems regardless of the adsorption sites. The hydrogen-vacancy substitutional site is found to be the most favourable for the adsorption of Cr and Fe, resulting in half metallic magnetic ground states with supercell magnetic moments of 5 μB and 3 μB respectively. On the contrary, the Mn adatom shows appreciable preference to adsorb on the top of a carbon atom, with large magnetic moment of 5 μB. The observed half metallicity and the rich magnetic properties of these systems are particularly important for efficient spin injection and transport of high spin polarized currents, desirable in spintronic device applications.

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