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Noble Metals and Transition Metals Adsorbed on Graphene: The Pursuit of Graphene Spintronics MATHEUS PAES LIMA, Univeristy of Sao Paulo, ADALBERTO FAZZIO, University of Sao Paulo — Via first-principles simulations we study the structural, magnetic and electron transport properties of 2D graphene in the presence of single atoms. We consider Cu, Ag and Au, as well as Mn, Fe, Co and Ni adsorbed on pristine and defective graphene containing vacancies and divacancies. To obtain the transport properties we perform ab-initio calculations based on Density Functional Theory (DFT) coupled to Non-Equilibrium Greens' Function (NEGF) formalism using the Landauer-Büttiker formula within the Meir-Wingreen approach. Our results show that graphene+noble metals systems have a gate controllable spin polarized current, allowing the fabrication of switchable spin filters with a moderated efficiency. In the particular case of Gold adsorbed on pristine graphene, a positive gate leads to a polarized current with excess of up electrons, while a negative gate the converse. Despite the high-spin configuration of Mn, the d levels are very far from the Fermi level. The Ni atom prefers a non-magnetic configuration. Therefore, graphene+transition metals systems present a polarized current only for Fe and Co atoms, allowing the fabrication of spin filters with very high efficiency.

Matheus Paes Lima
University of Sao Paulo

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