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Non-equilibrium Transport in Carbon based Adsorbate Systems
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We have used the Atomistix Tool Kit(ATK) and TranSIESTA[1] packages to investigate adsorption of iron atoms on a graphene sheet. The technique of both codes is based on density functional theory using local basis sets[2], and non-equilibrium Green's functions (NEGF) to calculate the charge distribution under external bias. Spin dependent electronic structure calculations are performed for different iron coverages. These reveal adsorption site dependent charge transfer from iron to graphene leading to screening effects. Transport calculations show spin dependent scattering of the transmission which is analysed obtaining the transmission eigenchannels for each spin type. The phenomena of electromigration of iron in these systems at finite bias will be discussed, estimating the so-called wind force from the reflection[3]. [1] M. Brandbyge, J.-L. Mozos, P. Ordejon, J. Taylor, and K. Stokbro. Physical Review B (Condensed Matter and Materials Physics), 65(16):165401/11-7, 2002. [2] Jose M. Soler, Emilio Artacho, Julian D. Gale, Alberto Garcia, Javier Junquera, Pablo Ordejon, and Daniel Sanchez-Portal. Journal of Physics Condensed Matter, 14(11):2745-2779, 2002. [3] Sorbello. Theory of electromigration. Solid State Physics, 1997.

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