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Chemically Tunable Transport Phenomena of Functionalized Graphene NICOLAS LECONTE, AURÉLIEN LHERBIER, FRANCOIS VARCHON, JEAN-CHRISTOPHE CHARLIER, Universite Catholique de Louvain, Institut de la Matiere Condensee et des Nanosciences (IMCN), NAPS-ETSF, Belgium, JUAN JOSE PALACIOS, ICREA, Institucio Catalana de Recerca i Estudis Avançats, Spain, DAVID SORIANO, PABLO ORDEJON, STEPHAN ROCHE, CIN2 (ICN-CSIC) and Universitat Autonoma de Barcelona, Catalan Institute of Nanotechnology, Spain — We present an ab initio multiscale study and quantum transport simulations using the Kubo formalism [1] of chemically modified graphene based materials, whose properties are tuned by changing the density and nature of grafted molecular units. Depending on the nature of the introduced molecular bonding different conduction mechanism are obtained, including transition from weak to strong Anderson localization [2,3], as well as spin-dependent phenomena [4] and magnetoresistive fingerprints [5].

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