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Tailoring Graphene Spintronics from first Principles[1] IGOR ZUTIC, University at Buffalo, PREDRAG LAZIC, Rudjer Boskovic Institute, GUILHERME MATOS SIPAHI, University at Buffalo, Universidade de Sao Paulo, NICOLAE ATODIRESEI, Peter Grunberg Institut, ROLAND KAWAKAMI, Ohio State University, KIRILL BELASCHENKO, University of Nebraska, Lincoln, BRANISLAV NIKOLIC, University of Delaware — Graphene/ferromagnet junctions provide large spin signals and important opportunities for spintronic devices [1,2]. However, for critical studies of such structures it is crucial to establish accurate predictive methods that would yield atomically-resolved information of interfacial properties and incorporate van der Walls interactions. We formulate a computationally-inexpensive model to study spin injection and proximity effects [3] and apply our finding to magneto-logic gates [2] using Ni(111) or Co(0001) as the ferromagnetic electrode. We show that spin polarization maps can be a versatile tool to tailor materials properties for graphene spintronics and explore their relation to computationally more demanding nonequilibrium transport codes [4]. [1] W. Han et al., Phys. Rev. Lett. 105, 167202 (2010); I. Neumann et al., Appl. Phys. Lett. 103,112401 (2013). [2] H. Dery et al., IEEE Trans. Electron Dev. 59, 259 (2012). [3] G. M. Siphai et al., J. Phys. Cond. Matter (in press); P. Lazic et al., preprint. [4] K. K. Saha, et al., Phys. Rev. B 85, 184426 (2012).

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