Abstract Submitted
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Six-band nearest-neighbor tight-binding model for the π-bands of bulk graphene and graphene nanoribbons[1] TIMOTHY BOYKIN, The University of Alabama in Huntsville, MATHIEU LUISIER, Integrated Systems Laboratory, GERHARD KLIMECK, Purdue University, XUEPING JIANG, NEERAV KHARCHE, YU ZHOU, SAROJ NAYAK, Rensselaer Polytechnic Institute (RPI), RPI COLLABORATION — The commonly used single-p_z orbital first nearest-neighbor tight-binding model faces two main problems: (i) it fails to reproduce asymmetries in the bulk graphene bands; (ii) it cannot provide a realistic model for hydrogen passivation of the edge atoms. As a result, some armchair graphene nanoribbons (AGNRs) are incorrectly predicted as metallic. A new nearest-neighbor, three orbital per atom p/d tight-binding model [1] is built to address these issues. The parameters of the model are fit to bandstructures obtained from first-principles density-functional theory and many-body perturbation theory within the GW approximation, giving excellent agreement with the ab initio AGNR bands. This model is employed to calculate the current-voltage characteristics of an AGNR MOSFET and the conductance of rough-edge AGNRs, finding significant differences versus the single-p_z model. Taken together these results demonstrate the importance of an accurate and computational efficient band structure model for predicting the performance of graphene-based nanodevices. [1] T. B. Boykin, M. Luisier, G. Klimeck, X. Jiang, N. Kharche, Y. Zhou and S. Nayak, J. Appl. Phys. 109, 104304 (2011)

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