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New Computational Approach to Electron Transport in Irregular Graphene Nanostructures DOUGLAS MASON, ERIC HELLER, Physics Dept., Harvard University, Cambridge, MA, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA — For novel graphene devices of nanoscale-to-macroscopic scale, many aspects of their transport properties are not easily understood due to difficulties in fabricating devices with regular edges. Here we develop a framework to efficiently calculate and potentially screen electronic transport properties of arbitrary nanoscale graphene device structures. A generalization of the established recursive Green's function method is presented, providing access to arbitrary device and lead geometries with substantial computer-time savings. Using single-orbital nearest-neighbor tight-binding models and the Green's function-Landauer scattering formalism, we will explore the transmission function of irregular two-dimensional graphene-based nanostructures with arbitrary lead orientation. Prepared by LBNL under contract DE-AC02-05CH11231 and supported by the U.S. Dept. of Energy Computer Science Graduate Fellowship under grant DE-FG02-97ER25308.

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