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Identification of nucleobases using variable currents through graphene nanopores: A first principles study J.T. HARALDSEN, Department of Physics and Astronomy, James Madison University, H. MCFARLAND, Department of Biology, James Madison University, T. AHMED, Theoretical Division, Los Alamos National Laboratory, J.-X. ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — Nanopore-based technology has the potential to be an efficient method for DNA/RNA base sequencing, as well as an identifier of other biomolecules. However, the thickness of the nanopore substrate is critical for the identification of individual nucleobases due to resulting noise and resolution problems. Recently, graphene has been suggested as a possible nanopore substrate due to its single atomic thickness and robust strength. In this study, we examine a possible device mechanism for the voltage dependence of nucleobases passing through a graphene nanopore. We utilize density functional theory with a generalized gradient approach on a graphene ribbon with a nucleobase in order to calculate the transmission spectra for each base. Transmission spectra for each base allows for the calculation of the ballistic current and differential current as a function of voltage. We show that applying various bias voltages across a graphene ribbon for the general, energy-minimized position of the translocated nucleobase, it is possible to distinguish individual bases using the resulting current. Overall, our goal is to improve nanopore device design by helping to further DNA/RNA nucleobase identification and sequencing.

Jason Haraldsen
James Madison University

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