Abstract Submitted
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Ab initio **Calculations of Electronic Fingerprints of DNA bases on Graphene**[1] TOWFIQ AHMED, JOHN J. REHR, Univ. of Washington, SVETLANA KILINA, North Dakota State University, TANMOY DAS, JASON T. HARALDSEN, ALEXANDER V. BALATSKY, Los Alamos National Laboratory — We have carried out first principles DFT calculations of the electronic local density of states (LDOS) of DNA nucleotide bases (A,C,G,T) adsorbed on graphene using LDA with ultra-soft pseudo-potentials. We have also calculated the longitudinal transmission currents $T(E)$ through graphene nano-pores as an individual DNA base passes through it, using a non-equilibrium Green's function (NEGF) formalism. We observe several dominant base-dependent features in the LDOS and $T(E)$ in an energy range within a few eV of the Fermi level. These features can serve as electronic fingerprints for the identification of individual bases from dI/dV measurements in scanning tunneling spectroscopy (STS) and nano-pore experiments. Thus these electronic signatures can provide an alternative approach to DNA sequencing.

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