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From frontier states to an inter-nucleotide potential for DNA: a density functional theory based study MARIA FYTA, Department of Physics, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics and School of Engineering and Applied Sciences, Harvard University — We present results from accurate density functional theory based simulations of individual DNA bases and representative base-pairs in various relative configurations, as they are likely to appear in the equilibrium and stretched forms of DNA. Specifically, we extract the salient features of electronic structure of these molecules and reveal that the frontier states in the base pairs are related to only one component of the pair. For all combinations of bases and base pairs studied here, the nature of these states was not affected by separation of the bases or base pairs along different directions or rotation along the helical axis. From the same calculations we were able to parametrize and construct an optimized intermolecular potential for DNA nucleotides, that accounts for hydrogen bonding, stacking interactions and the contribution from the sugar backbone. These calculations serve to set the stage for more extensive coarse grain calculations of DNA related biophysical phenomena.

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