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Electronic Structure of DNA: A Maximally-Localized Wannier Function Approach ARASH MOSTOFI, NICOLA MARZARI, Massachusetts Institute of Technology — We combine large-scale, *ab initio* electronic structure calculations and the maximally-localized Wannier function approach in order to study the electronic properties of DNA strands. By performing full first-principles calculations on stacked DNA base-pairs, we determine the optimally localized, real-space basis set that is able to describe the infinite one-dimensional system efficiently and accurately. This work opens the way to obtaining a detailed understanding of charge transport and conductance in DNA, bringing closer the prospect of engineering its electronic structure for use in nano-electronic circuits and biotechnology applications.

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