Abstract Submitted
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Quasiparticle properties of DNA bases from GW calculations in a Wannier basis XIAOFENG QIAN, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, PAOLO UMARI, Theory at Elettra Group, CNR-INFM Democritos, Basovizza (Trieste), Italy — The quasiparticle GW-Wannier (GWW) approach [1] has been recently developed to overcome the size limitations of conventional planewave GW calculations. By taking advantage of the localization properties of the maximally-localized Wannier functions and choosing a small set of polarization basis we reduce the number of Bloch wavefunctions products required for the evaluation of dynamical polarizabilities, and in turn greatly reduce memory requirements and computational efficiency. We apply GWW to study quasiparticle properties of different DNA bases and base-pairs, and solvation effects on the energy gap, demonstrating in the process the key advantages of this approach. [1] P. Umari,G. Stenuit, and S. Baroni, cond-mat/0811.1453

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