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Computing quasiparticle energies and band offsets for large systems[1] MARCO GOVONI, Department of Chemistry, University of California Davis, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — We present a massively parallel implementation [1] of a method [2] recently proposed for the calculations of quasiparticle energies of molecules and solids, which does not require the explicit evaluation of single particle virtual states. Explicit inversion and storage of large dielectric matrices are also avoided and frequency integration is explicitly carried out, without resorting to plasmon pole models. We present application to complex semiconducting interfaces, inclusive of order and disordered systems, with more than one thousand electrons.
[1] M. Govoni and G. Galli, in preparation.
[2] H-V. Nguyen et al. Phys. Rev. B 85, 081101(R) (2012); T.A. Pham et al. Phys Rev. B 87, 155148 (2013)

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