Abstract Submitted
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Faster GW total energy calculations[1] MZURI HANDLIN, MARCO GOVONI, GIULIA GALLI, University of Chicago, Institute for Molecular Engineering — Accurate calculations of total energies are necessary for understanding and predicting material properties. Currently density functional theory is the most widely used method for condensed systems, but in most cases it cannot accurately treat systems with dispersion interactions. Many body perturbation theory within, e.g. the GW approximation (GW), may in principle treat dispersion interactions accurately, but at a high computational cost. A major bottleneck of standard GW calculations is the required storage and inversion of large dielectric matrices, as well as the determination of their frequency dependence; the recently developed projective dielectric eigenpotential (PDEP) algorithm together with Lanczos based techniques [2,3] avoid these problems by using a spectral decomposition of the dielectric matrix. We generalized the PDEP algorithm to efficiently compute GW total energies and we will present results for the energies of molecular crystals and solids of nanoparticles.

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[2]T. Pham, H. Nguyen, D. Rocca and G. Galli, Phys. Rev. B 87, 155148 (2013)
[3]M. Govoni and G. Galli, Large scale GW calculations, submitted

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