

Abstract Submitted
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Verification and Validation of GW calculations for solids IKUTARO HAMADA, National Institute for Materials Science, MARCO GOVONI, Materials Science Division, Argonne National Laboratory and Institute for Molecular Engineering, University of Chicago and , GIULIA GALLI, Institute for Molecular Engineering, University of Chicago and Materials Science Division, Argonne National Laboratory — Many body perturbation theory based on the GW approximation is a well established approach to compute quasiparticle energies of solids. Yet, systematic convergence tests as a function of basis sets, k-points and other numerical parameters entering the calculation are still lacking. We present a systematic convergence study of quasiparticle energies using a new release of the large-scale GW code WEST[1,2] including accurate k-point sampling of the Brillouin zone[3]. We also discuss comparisons with experiments.

[1] M. Govoni and G. Galli, J. Chem. Theory Comput. 11, 2680 (2015); www.west-code.org

[2] P. Scherpelz, M. Govoni, I. Hamada and G. Galli J. Chem. Theory Comput. 12, 3523 (2016).

[3] I. Hamada, M. Govoni and G. Galli (to be published).

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