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Cubic scaling GW: towards fast quasiparticle calculations PEITAO LIU, MERZUK KALTAK, University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria, JIŘí KLIMEŠ, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejškova 3, CZ-18223 Prague 8, Czech Republic, GEORG KRESSE, University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — Within the framework of the full potential projector-augmented wave methodology, we present a promising low-scaling GW implementation. It allows for quasiparticle calculations with a scaling that is cubic in the system size and linear in the number of k points used to sample the Brillouin zone. This is achieved by calculating the polarizability and self-energy in real space and imaginary time. The transformation from the imaginary time to the frequency domain is done by an efficient discrete Fourier transformation with only a few nonuniform grid points. Fast Fourier transformations are used to go from real space to reciprocal space and vice versa. The analytic continuation from the imaginary to the real frequency axis is performed by exploiting Thiele's reciprocal difference approach. Finally, the method is applied successfully to predict the quasiparticle energies and spectral functions of typical semiconductors (Si, GaAs, SiC, and ZnO), insulators (C, BN, MgO, and LiF), and metals (Cu and $SrVO_3$). The results are compared with conventional GW calculations. Good agreement is achieved, highlighting the strength of present method.

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