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Low scaling algorithms for the random phase and *GW* approximation[1] MERZUK KALTAK, JIRI KLIMES, GEORG KRESSE, University of Vienna, Faculty of Physics and Center for Computational Materials Science — The computationally most expensive step in conventional RPA implementations is the calculation of the independent particle polarizability χ_0. We present an algorithm that calculates χ_0 using the Green's function in real space and imaginary time. In combination with optimized non-uniform frequency and time grids the correlation energy on the random phase approximation level can be calculated efficiently with a computational cost that grows only cubically with system size [1,2]. We apply this approach to calculate RPA defect energies of silicon using unit cells with up to 250 atoms and 128 CPU cores. Furthermore, we show how to extent the algorithm to the *GW* framework of Hedin and solve the Dyson equation for the Green's function with the same computational effort.

[1] M. Kaltak, J. Klimeš, and G. Kresse, Journal of Chemical Theory and Computation 10, 2498-2507 (2014).
[2] M. Kaltak, J. Klimeš, and G. Kresse, Phys. Rev. B 90, 054115 (2014).

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