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Efficient GW methods implemented in molecular orbital space: Ionization energy and electron affinity of conjugated molecules[1] SAN-HUANG KE, Department of Physics, Tongji University, 1239 Siping Road, Shanghai 200092, China — An efficient all-electron non-selfconsistent GW (G^0W^0) method is proposed, which is based on the full random-phase approximation and implemented in the molecular-orbital space with algorithms for reducing the error coming from the incompleteness of the basis set. The convergence of its result with regard to the size of the basis set is examined. Based on this, we further implement a quasiparticle self-consistent GW (QSGW) approach with Gaussian basis functions. The high computational efficiency allows us to deal with larger molecules from the first principles, and we applied our methods to calculate the ionization energy (IE) and electron affinity (EA) of ten conjugated molecules with up to 32 atoms. The G^0W^0 result improves the Hartree-Fock result significantly, especially for EA, and, furthermore, the QSGW improves the G^0W^0 and gives results of both IE and EA in very good agreement with the available experimental data and also with the results from the ΔSCF calculation using the B3LYP functional. This indicates that our all-electron *ab initio* GW calculation can describe very well molecular electronic structures, making the QSGW approach a good candidate for investigating electronic and transport properties of molecular systems.

San-Huang Ke
Department of Physics, Tongji University,
1239 Siping Road, Shanghai 200092, China

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