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Ab initio calculations of quasiparticle energies of solids, liquids and molecules using a spectral decomposition of the dielectric matrix¹ TUAN ANH PHAM, Department of Chemistry UC Davis and Lawrence Livermore National Laboratory, HUY-VIET NGUYEN, Institute of Physics, Hanoi, Vietnam, DARIO ROCCA, Department of Chemistry, UC Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — We recently developed a method for the calculation of quasiparticle energies within many body perturbation theory, at the GW level, which avoids costly summations over empty electronic states and does not require the use of plasmon-pole models [1]. We present a comprehensive validation of this method, encompassing calculations of i) the vertical ionization energies of a set of over 80 molecules (containing from 14 to 424 valence electrons); ii) the relative position of energy levels of anions and water in hydrated sulfate and chloride clusters; iii) the band structure of a variety of semiconductors and (iv) the electronic properties of amorphous and liquid systems. The efficiency of our approach allowed us to compute quasiparticle energies of multiple configurations of liquid water, using samples with 64 molecules, selected over trajectories generated by ab initio molecular dynamics simulations.

[1] H. Viet Nguyen, T. Anh Pham, D. Rocca and G. Galli, Phys. Rev. B 85, 081101(R) (2012); T. Anh Pham, H. Viet Nguyen, D. Rocca and G. Galli (submitted)

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