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Probing the electronic structure of liquid water with many-body perturbation theory[1] TUAN ANH PHAM, Department of Chemistry UC Davis and Lawrence Livermore National Laboratory, CUI ZHANG[2], Department of Chemistry UC Davis, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — We present a first-principles investigation of the electronic structure of liquid water based on many-body perturbation theory (MBPT), within the G_0W_0 approximation. The liquid quasiparticle band gap and the position of its valence band maximum and conduction band minimum with respect to vacuum were computed and it is shown that the use of MBPT is crucial to obtain results that are in good agreement with experiment. We found that the level of theory chosen to generate molecular dynamics trajectories may substantially affect the electronic structure of the liquid, in particular, the relative position of its band edges and redox potentials. Our results represent an essential step in establishing a predictive framework for computing the relative position of water redox potentials and the band edges of semiconductors and insulators.

[1] T. Anh Pham, C. Zhang, E. Schwegler and G. Galli (submitted).

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