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Ab initio calculation of optical spectra of solvated molecules: GW+BSE method for liquid environments JEEHYE LEE, TOMAS ARIAS, Cornell University — Electronic excitations for solvated systems have drawn a great interest in the energy community because they provide a possibility to engineer photoexcitation processes. Time-dependent DFT (TDDFT) and the hybrid QM/MM approach successfully calculate the solvent shift in excitation energies (solvatochromic shift) for confined systems, but are well known to work best for small systems and Frenkel excitons. Here we present a new modification of the GW and Bethe-Salpeter equation (GW+BSE) methods which allows treatment of solvated systems beyond the TDDFT level by including the frequency-dependent polarizability of the solvent at the diagrammatic level. In this initial work, we present the solvatochromic and ionization potential shifts for a series of molecules in aqueous solution.

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