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Efficient GW calculations using eigenvalue-eigenvector decomposition of the dielectric matrix[1] HUY-VIET NGUYEN, T. ANH PHAM, DARIO ROCCA, GIULIA GALLI, University of California-Davis — During the past 25 years, the GW method [1] has been successfully used to compute electronic quasiparticle excitation spectra of a variety of materials. It is however a computationally intensive technique, as it involves summations over occupied and empty electronic states, to evaluate both the Green function (G) and the dielectric matrix (DM) entering the expression of the screened Coulomb interaction (W). Recent developments have shown that eigenpotentials of DMs can be efficiently calculated without any explicit evaluation of empty states [2]. In this work, we will present a computationally efficient approach to the calculations of GW spectra by combining a representation of DMs in terms of its eigenpotentials [3] and a recently developed iterative algorithm [4]. As a demonstration of the efficiency of the method, we will present calculations of the vertical ionization potentials of several systems. [1] L. Hedin, Phys. Rev. 139, A796 (1965). [2] H.-V. Nguyen and S. de Gironcoli, Phys. Rev. B 79, 205114 (2009); H. F. Wilson, D. Lu, F. Gygi, and G. Galli, Phys. Rev. B 79, 245106 (2009). [3] D. Lu, F. Gygi, and G. Galli, Phys. Rev. Lett. 100, 147601 (2008). [4] P. Umari, G. Stenuit, and S. Baroni, Phys. Rev. B 81, 115104 (2010)

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Viet Nguyen
University of California-Davis

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