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New *ab initio* approaches for calculating the microscopic electron-density response matrix KATHLEEN SCHWARZ, Cornell University Department of Chemistry, JEEHYE LEE, T.A. ARIAS, Cornell University, Department of Physics — The electron-density response matrix is a key quantity for excitation calculations such as GW-BSE. Typically, the response matrix is obtained at the level of the random phase approximation (RPA), with the wavefunction from local density approximation (LDA) density functional theory. The expense of this approach grows quickly with the number of atoms, and its accuracy depends on both the accuracy of the LDA and the RPA. We investigate a series of approaches to overcome these difficulties, based on an eigenvalue decomposition of the molecular response matrix.

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