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Efficient calculation of random-phase approximation correlation energies using Lanczos chains and an optimal basis set DARIO ROCCA, Université de Lorraine and CNRS, Nancy (France) — A new *ab initio* approach is introduced to compute the correlation energy within the adiabatic connection fluctuation dissipation theorem in the random phase approximation. First, an optimally small basis set to represent the response functions is obtained by diagonalizing an approximate dielectric matrix containing the kinetic energy contribution only [1]. Then, the Lanczos algorithm is used to compute the full dynamical dielectric matrix and the correlation energy [1,2]. The convergence issues with respect to the number of empty states or the dimension of the basis set are avoided and the dynamical effects are easily kept into account. To demonstrate the accuracy and efficiency of this approach the binding curves for three different configurations of the benzene dimer are computed: T-shaped, sandwich, and slipped parallel.

[1] D. Rocca, J. Chem. Phys. (2014), to appear in the special issue Advances in DFT Methodology.
[2] T.A. Pham, H.-V. Nguyen, D. Rocca, G. Galli, Phys. Rev. B 87, 155148 (2013).

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