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Long range correlation energy from coupled atomic response functions ALBERTO AMBROSETTI, ALEXANDRE TKATCHENKO, Fritz-Haber Institute — Electron correlation is an elusive and ubiquitous energy contribution that arises from transient many-body electron excitations. Its reliable (accurate and efficient) modeling is essential for correctly describing cohesive, structural, and response properties of molecules and solids. In this regard, the main challenge is to model the long-range correlation energy beyond (semi-)local density-functional approximations. Here we propose an efficient method to compute the long-range correlation energy for non-metallic molecules and solids, by using coupled atomic response functions (ARF). Extending the recent MBD method [1], we separate the coupling between ARFs into short and long range, allowing seamless treatment of weakly and strongly polarizable systems. Thorough benchmarking on large data sets including small molecules (S22, S66x8), supramolecular complexes (S12L), molecular crystals (X23) and graphite shows consistently good agreement with high level theoretical and experimental reference data (of the order of 6%). The uniform accuracy for molecules and solids represents a strong validation of our method, and further confirms the importance of modeling the truly collective nature of the long-range correlation energy. [1] A. Tkatchenko et al. PRL **108** 236402 (2012).

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