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Excitation gaps of finite-sized systems from Optimally-Tuned Range-Separated Hybrid Functionals[1]

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Excitation gaps are of much significance in electronic structure theory. Within many-body perturbation theory, the fundamental gap is the difference between the lowest quasi-hole and quasi-electron excitation energies and the optical gap is addressed by including the quasi-electron - quasi-hole interaction. A long-standing challenge has been the attainment of a similar description within density functional theory (DFT), with much debate on whether this is achievable even in principle. Here, I describe a new DFT approach to this problem. Anchored in the generalized Kohn-Sham framework, our method is based on a range-split hybrid functional with exact long-range exchange. Its novel feature is that the range-splitting parameter is determined from first principles, per-system, based on satisfaction of physical constraints. For finite objects, this approach mimics successfully the quasi-particle excitation picture. It allows the extraction of the fundamental and optical gap from one underlying functional, based on the ground-state HOMO-LUMO gap and the lowest excitation of linear-response time-dependent DFT, respectively. It is equally accurate for the difficult case of charge-transfer excitations and it produces accurate outer-valence simulated photoelectron spectra.

[1]Work with many students and co-workers, especially the groups of R. Baer (Hebrew U) and J. B. Neaton (Berkeley) is greatly appreciated