

Myopia Under the Microscope

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We previously presented a technique to measure the spatial dependence of electron correlation effects present in the doubles amplitudes under the least-squares tensor hypercontraction (LS-THC) approximation. This approach probes both the energetic and geometric properties of “basis functions” comprised of pairs of spatial grid points, and highlights the location and length scale of non-local electronic interactions in molecules. In this talk, we extend our analysis to a rich data set and uncover a number of interesting features about the LS-THC-decomposed doubles amplitudes which are highly consistent across basis sets, electronic structure methods, and molecular systems. We also examine the LS-THC decomposition of the excited state double amplitudes in the equation-of-motion coupled cluster theory and explore how spatial signatures of electronic interactions differ between the ground and excited states.