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Triplet Pairing and Odd-Electron Densities in Constrained-Pairing Mean-Field Theory JASON K. ELLIS, Department of Physics and Astronomy and Department of Chemistry, Rice University, CARLOS A. JIMENEZ-HOYOS, Department of Chemistry, Rice University, GUSTAVO E. SCUSERIA, Department of Chemistry and Department of Physics and Astronomy, Rice University — Describing strong (also known as static or non-dynamical) correlation caused by degenerate or nearly degenerate orbitals near the Fermi level remains a theoretical challenge, particularly in molecular systems. Constrained-pairing mean-field theory (CPMFT) has been quite successful capturing the effects of static correlation in bond formation and breaking in closed-shell molecular systems. This method uses singlet electron entanglement to model static correlation at *mean field* cost. The present work extends the previous formalism to include triplet pairing, allowing a description of same-spin correlation and open-shell species. Additionally, a spin-orbital extension of the “odd-electron” formalism of Yamaguchi and co-workers is presented as a method for understanding triplet radical character in molecules. Results from representative systems are presented.

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