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Magnetism-Tuning Strategies of Graphene Oxide: Based on Theoretical Simulation of Magnetic Oligoacene Oxide Patches

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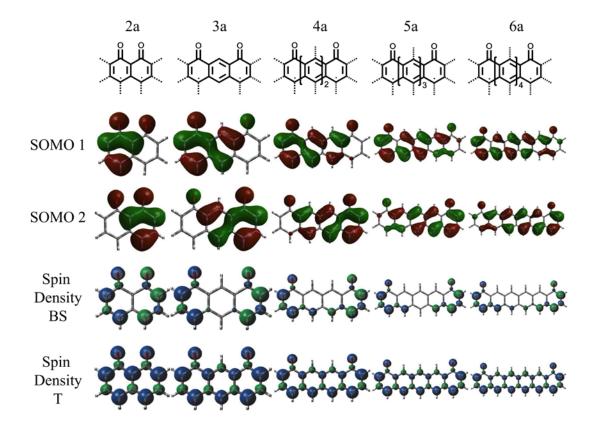


Figure S1 Topological representation of different series of a-series diradicals, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.

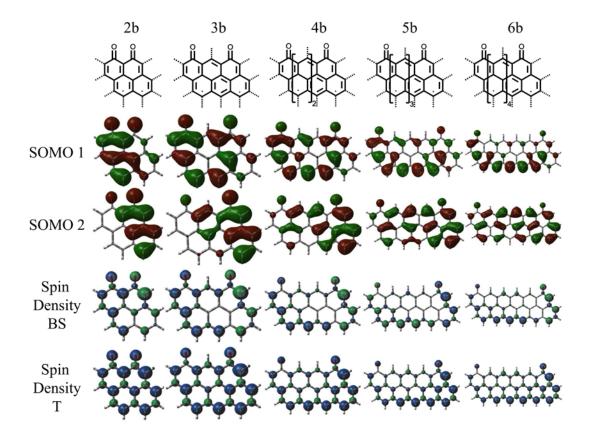


Figure S2 Topological representation of different series of b-series diradicals, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.

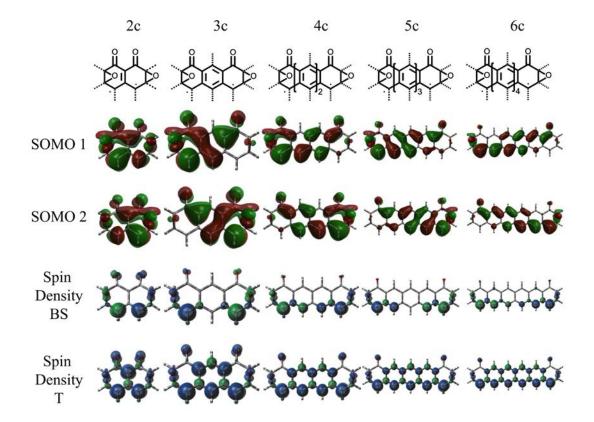


Figure S3 Topological representation of different series of c-series diradicals, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.

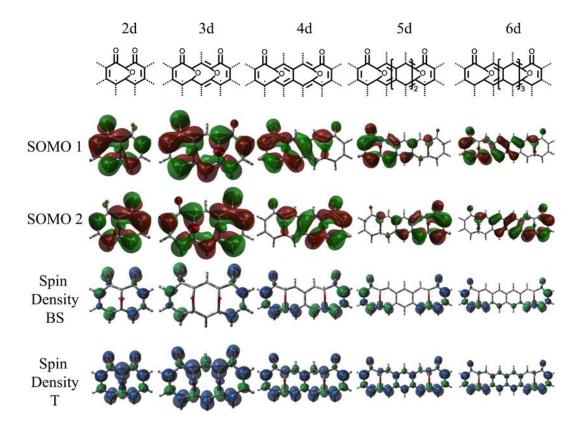


Figure S4 Topological representation of different series of d-series diradicals, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.

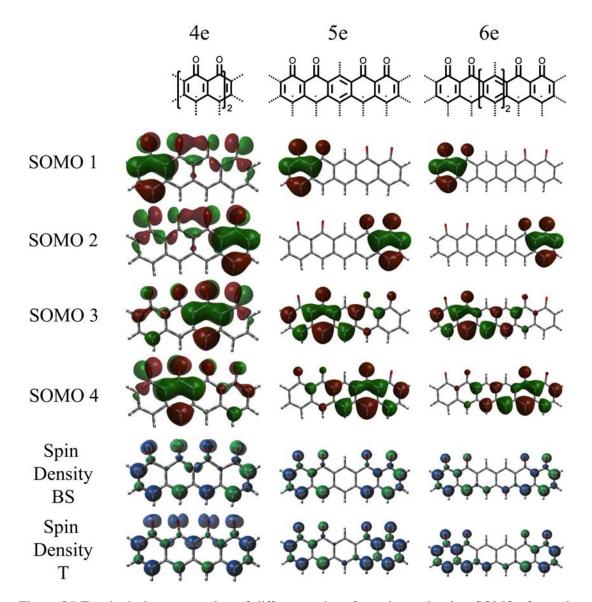


Figure S5 Topological representation of different series of e-series molecules, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.

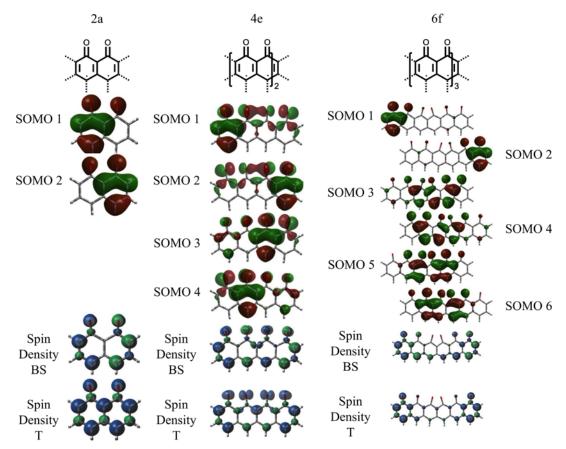


Figure S6 Topological representation of different series of 2a, 4e and 6f, SOMOs for each radical, distribution of the spin densities of BS (open-shell broken-symmetry) state and T (triplet) state.