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The Nature of Binding in the Phenalenyl Dimer and its Derivatives BRIAN KOLB, TIMO THONHAUSER, Wake Forest University, MIKLOS KERTESZ, Georgetown University — The biradical phenalenyl π-dimer and its derivatives have attracted interest recently because of their potentially useful electrical, optical, and magnetic properties. These properties can be tuned by adjusting the binding characteristics between the monomers within the dimer. Typically, this is done by substituting electron withdrawing or donating groups onto the α or β-site carbons. An understanding of this binding lies at the heart of useful application of these materials. In this work, the binding characteristics of phenalenyl dimers were investigated using density functional theory. In particular, the vdW-DF functional was used to explore the role of van der Waals interactions in the binding within this system. A comparison of the binding curves with those of the closed shell derivatives wherein the central carbons have been replaced by either nitrogen or boron sheds light into the nature of the interactions between the monomers.

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