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Defect-Stabilized Graphene-Based Organometallic Sandwich Structures PRATIBHA DEV, THOMAS REINECKE, Naval Research Laboratory, Washington, D.C. — Benzene-transition metal-graphene (Bz—M—Gr) sandwich structures are of interest in a range of applications such as catalysis, spintronics and quantum computing. Although they are predicted to form in several theoretical works, it has proven harder to create these complexes experimentally. Using density functional theory, we propose a chemical route to creating stable Bz—M—Gr sandwich structures. Acceptor-type defects, such as carbon vacancies and pyridinic nitrogen substituents in graphene are used to immobilize the metal onto graphene. Placing a benzene ring atop the metal atom further stabilizes the structure against oxidation. Structural, electronic and magnetic properties of the Bz—M—Gr complexes vary for different defects. High cohesive energies and spin polarization energies make defect-stabilized Bz—M—Gr complexes of interest for use as nanomagnets in ambient conditions.

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