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A Planar, Semiconducting Graphene Allotrope[1] DAVID APPELHANS, ZHIBIN LIN, MARK LUSK, Colorado School of Mines — A number of graphene allotropes have been proposed which maintain a two-dimensional carbon structure while exhibiting interesting mechanical and electronic properties. In recent works, we have shown how these new carbon phases, pentaheptite, the haeckelites, and the dimerites, can be constructed from graphene using a combination of Stone-Thrower-Wales (STW) and Inverse Stone-Thrower-Wales (ISTW) defects. Significantly, all of these allotropes are metallic, and this limits the manner in which they might be incorporated into the emerging field of carbon electronics. Motivated by this, we have employed di-vacancies (DVs) as the third member of a defect alphabet to broaden the design space for technologically important carbon sheets. This has resulted in the identification of a metallic, planar graphene allotrope with a lower ground state energy than any previously identified. Even more important, though, is the computational discovery of a relatively low-energy, planar, semi-conducting allotrope. This material can be fabricated entirely from SW and DV defects and can also be created as both islands and ribbons within an existing graphene sheet. This offers the prospect of creating electronic components solely using graphene defect engineering. We employ a combination of density functional theory (DFT) and screened Green function (GW) theory to elucidate the structure and electronic properties of this new semiconductor.

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