

Abstract Submitted
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New Lowest Energy Graphene Allotropes Utilizing 8 Membered Defect Rings DAVID APPELHANS, MARK LUSK, Colorado School of Mines — The combination of Stone-Thrower-Wales (STW) and the recently identified Inverse-Stone-Thrower-Wales (ISTW) defects in graphene allow a wide range of graphene allotropes to be constructed. This is accomplished by applying combinations of these defects in a periodic template on pure graphene. For instance, the three lowest energy Haeckelite structures can be constructed in this way as has a new class of low energy graphene allotropes, Dimerites, which use only ISTW defects. All of these Haeckelites and Dimerites, though, are composed of 5-, 6-, and 7-membered rings. We have focused on 8-membered rings and predict a new family of carbon allotropes. One of these, Appelite R568, is only 194 meV/atom higher in energy than graphene. This is the lowest energy graphene derivative predicted. We outline a pathway of defect creation leading to the structure.

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