

Abstract Submitted  
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**Size-dependence of electronic and optical properties of armchair graphene nanoislands**<sup>1</sup> JONATHAN MOUSSA, JAMES CHELIKOWSKY, UT Austin — Atomically precise armchair graphene nanoislands (benzenoid polycyclic aromatic hydrocarbons) have been produced by organic synthesis and to-date have attained sizes up to 222 carbon atoms. The electronic and optical properties of these nanoislands are studied using a combination of semi-empirical methods, time-dependent density functional theory, and the GW/Bethe-Salpeter formalism. Comparisons are made with experimental measurements where available. For this class of materials, theory is able to predict the necessary nanoisland sizes required for potential photovoltaic and light-emitting applications. The study of large nanoislands is focused on parallelogram-shaped islands, which should be particularly amenable to synthesis over a wide range of sizes.

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