

# From Zero to Infinity: Customized Atomistic Calculations for Crystalline Solids — Applications to Graphene and Diamond

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1) The expanded “main sequence PAHs

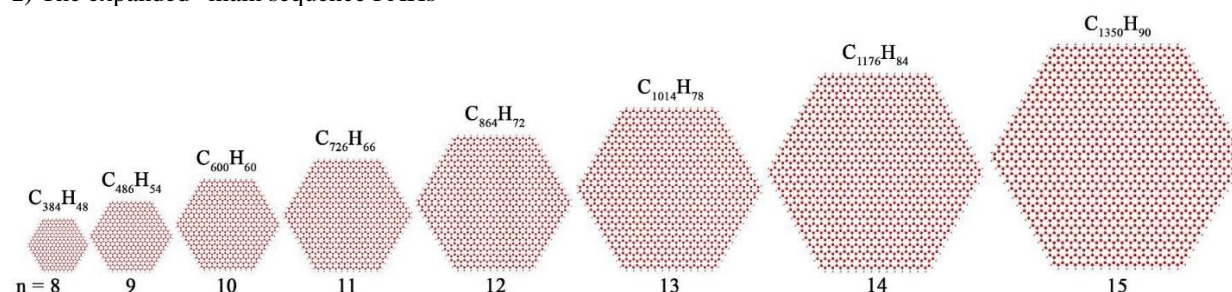


Fig. S1. The main sequence PAHs for shell numbers  $n = 8$  up to  $n = 15$

2) The HOMO, LUMO Molecular orbitals for the 9<sup>th</sup> and 14<sup>th</sup> PAHs

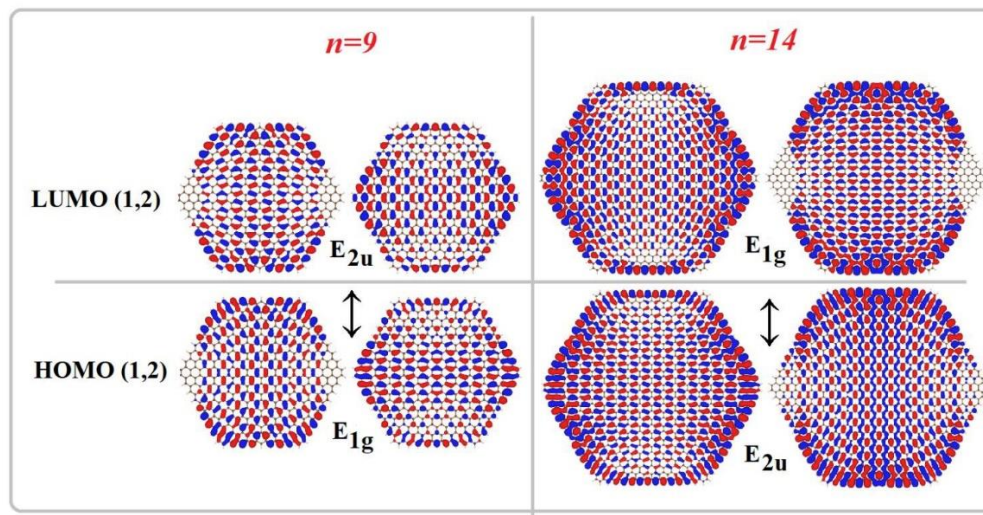


Fig. S2. The HOMO (1, 2) and LUMO (1, 2) molecular orbitals for the odd shell number 9, and the even shell number 14. Isovalues = 0.01 and 0.005 respectively.

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## 3) The Full reference 34

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