Abstract Submitted

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Geometrical structures and electronic properties of Sm, K-doped chrysene XIAO-HUI WANG, Beijing Computational Science Research Center, Beijing, 100094, China, GUO-HUA ZHONG, Center for Photovoltaics and Solar Energy, Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, Shenzhen, 518055, China —The discovery of superconductivity in potassium-doped picene ($K_xC_{22}H_{14}$) has revitalized the research interest in polycyclic aromatic hydrocarbons (PAHs), and a large variety of PAHs superconductors have been reported afterwards, such as phenanthrene, coronene and 1,2;8, 9-dibenzopentacene. Recently a new PAHs superconductor, Sm-doped chrysene, with Tc ~ 5 K was reported experimentally whose precise nature is still unknown. In this work, crystal structure search and electronic structure of A-doped chrysene, A_x-$C_{18}H_{12}$ (A=Sm, K), have been studied by the first-principles density-functional theory using the projector augmented wave method based on the generalized gradient approximation implemented in the VASP package. We also include the van der Waals (vdW) corrections in the calculations, thus clarifying the dopant atoms positions and crystal structures of doped superconducting chrysene. Our findings represent a significant step toward the understanding of superconductivity of PAHs.