

Abstract Submitted
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Prediction of Superconductivity in Potassium-Doped Benzene¹

HAI-QING LIN, Beijing Computational Science Research Center, GUOHUA ZHONG, Center for Photovoltaics and Solar Energy, Shenzhen Institutes of, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research — To explore underline mechanism for the superconducting phase in recent discovered aromatic hydrocarbons, we carry out the first-principles calculations on benzene, the basic and the simplest unit of the series and examine the structural and phase stability when doped by potassium, $K_xC_6H_6$, $x = 1, 2, 3$. We found that $K_2C_6H_6$ with the space group of $Pbca$ is the most stable phase with superconducting transition temperature T_c around 6.2K. Moreover, we argue that all existing hydrocarbons should have superconducting phase in the same range, $5K < T_c < 7K$, when doped by potassium atoms.

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