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Theoretical Studies on Recent Discovered Organic Superconductors

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时间：5月16日（星期四）15:00—16:40

地点：北京大学物理大楼中212教室

林海青，北京计算科学研究中心教授，1987年美国加州大学San Diego分校物理学博士．主要从事凝聚态物理和计算物理的研究。主要研究兴趣包括：强关联系统，量子纠缠和量子相变，以及多体系统的数值方法。

Abstract: In this talk, I report our recent study on the magnetic and pair binding properties in newly discovered polycyclic aromatic hydrocarbon (PAH) superconductors including alkali-metal-doped picene, coronene, phenanthrene, and dibenzopentacene. To gain a better understanding on magnetism and electron correlation in PAH, we have performed a systematic numerical investigation on the correlation effects and model the π-electrons on the carbon atoms of a single molecule by a one-orbital Hubbard model, in which the energy difference ϵ between carbon atoms with and without hydrogen bonds is taking into account. We demonstrate that the spin polarized ground state is realized for charged molecules in the physical parameter regions, which provides a reasonable explanation of local spins observed in PAHs. In alkali-metal-doped dibenzopentacene, our results show that electron correlation may produce an effective attraction between electrons for the charged molecule with one or three added electrons. We also propose a different doping pattern which may lead to higher transition temperature. Some results on the possible structure of PAH as functions of pressure and doing will be discussed.

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