Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Numerical study of the magnetic and pair binding properties in aromatic hydrocarbon superconductors[1] ZHONGBING HUANG, Department of Physics, Hubei University, CHAO ZHANG, HAIQING LIN, Beijing Computational Science Research Center — We performed a systematic numerical study of the magnetic and pair binding properties in recently discovered aromatic hydrocarbon superconductors, by using exact diagonalization and quantum Monte Carlo methods. The π-electrons on the carbon atoms of a single molecule are modelled by the one-orbital Hubbard model, which takes into account the energy difference between carbon atoms with and without hydrogen bonds. Our results show that the spin polarized ground state is realized for charged molecules in the physical parameter region. This provides a reasonable explanation of local spins observed in experiments. In alkali-metal-doped picene and phenanthrene, the pairing binding energy is always negative for different electron doping densities, suggesting that electron correlation has no contribution to the formation of Cooper pairs. However, a positive pair binding energy for the charged dibenzopentacene molecule with one or three added electrons indicates that electron correlation may produce an effective attraction between electrons.

[1]This work was supported by NSFC under Grants Nos. 11174072 and 91221103.

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Date submitted: 08 Nov 2012 Electronic form version 1.4