

Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics of Charles University has a pleasure to invite you to attend the seminar

on 15 December 2022 at 14:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Lecture hall F2



doc. Ing. Pavel Jelínek, Ph.D.

Institute of Physics, AS CR

On-surface synthesis and SPM characterization of polyradical PAHs with strong multireference character

Joined with Nanoseminar. Note different time and place.

The recent progress in on-surface synthesis enabled to form new molecular structures, which are not available by traditional organic chemistry in solution [1]. Special attention was paid synthesis of open shell polyaromatic hydrocarbons (PAH) showing interesting magnetic properties [2]. In this talk, we will provide a brief review of different strategies to introduce π -magnetism in PAHs including frustrated topology of bipartite lattice or electron-electron correlation [3]. We will introduce another alternative using electron-phonon coupling in 1D π -conjugated systems [4]. The most of the PAH molecules prepared so far had a biradical character, where the description of the electronic structure can be well understood using the single determinant mean field methods such as DFT. Recently, few examples of polyradical molecules with multireference character has been reported [5]. We will present unpublished data reporting synthesis of polyradical molecules with strong multireference character. Their electronic structure is analyzed using SPM technique including nickelocene functionalized probes as well as DMRG and CAS calculations which enables to describe properly the multireference states. First, we will discuss a triangulene-based molecule, where tetraradical character is introduced in combination of the e-e interaction as well as the frustrated topology. We will also discuss the effect of the pentagon defects on the electronic structure as well as coexistence of Kondo and spin excitation in defective molecules. In second part, we will describe polyradical PAH macrocycles with eight-to-ten unpaired electrons. This cyclic system features frustrated magnetism with a strong entanglement between unpaired spins. Therefore, it represents an example of spin liquid hosted in a single molecule.

[1] S. Clair and D. G. de Oteyza, Chemical Reviews 119, 4717 (2019).

[2] J. Li et al., Nature Communication 10, 200 (2019); N. Pavlicek et al., Nature Nanotechnology 12, 308 (2017); S. Mishra et al., Nature Nanotechnology 15, 22 (2019).



For more information follow: theory.kfkl.cz/seminars.php

If you wish to receive regular updates on forthcoming seminars, contact K. Carva (carva@karlov.mff.cuni.cz).

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[3] R. Ortiz et al., Nano Letters 19, 5991 (2019).

[4] H. Gonzalez-Herrero et al, Adv. Mat. 33, 2104495 (2021).

[5] Sh. Mishra et al., Nature 598, 287 (2021); J. Hieuille et al., Angewandte Chemie Int. Ed. 60, 25224 (2021).

