



Universidade Federal da Paraíba
Centro de Ciências Exatas e da Natureza
Programa de Pós-Graduação *Stricto Sensu* em Física

Ciclo de Colóquios 2018.2

Colóquio nº 2

“Multiferroicity on purely organic molecules”

RESUMO: Conjugated systems have complex behaviors when increasing the number of monomers, which is one of the reasons that makes long oligomers hard to be characterized by numerical methods. An example of this is fused-azulene, a molecule that has been reported to displays an increasing magnetic moment with system size. Once these molecules also present charge polarization, fused azulene are strong candidates to be an organic multiferroic material. We show that a simple second-order perturbation treatment of electronic correlations by means of Rayleigh-Schroedinger Perturbation Theory allow to accurately infer about the magnetic state of these long complex π -conjugated molecules. Based on these results we propose to simple, and computationally cheap, protocol to search for polycyclic hydrocarbon molecules that would exhibit magnetic polarization. In the illustrative exploration, we found two magnetic molecules with 34 carbon atoms ($C_{34}H_{20}$), these molecules are shorter than the smallest magnetic fused-azulene oligomer. We confirm the magnetic nature of these new molecules by Density Functional Theory calculations.

Profª. Dra. Alexandra Valentim PosDoc – UFPB

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