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Perylene diimide liquid crystals: A density functional study JEVERSON ARANTES, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil, MATHEUS LIMA, Instituto de Fisica, Universidade de Sao Paulo, CP 66318, 05315-970 Sao Paulo, SP, Brazil, ADALBERTO FAZZIO, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil, HONGJUN XIANG, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA, GUSTAVO DALPIAN, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil — Organic semiconductors (OSs) are getting each time more space in the field of electronic materials mainly due to its low manufacturing costs, the relative facility of manufacturing in the desired way. A model for the crystal structure of perylene diimide PPEEB has been proposed, partially based on experimental observations. In this structural model, we've performed an *ab initio* calculations on the electronic structure of this material. Due to the strongly localized nature of the Oxygen atoms on the side chains, is necessary to go beyond the standard LDA and GGA calculations. With the PBE0 approach, the electronic structure becomes in agreement with previous results. The tails of the molecular crystal not only is responsible for its structural conformation, but also can be used for tuning the electronic and optical properties of the material.

Jeverson Arantes
Universidade Federal do ABC

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