Poster Presentation

MS25.P03

Modeling of the optical properties of molecular crystals

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In this contribution we present our current findings in the calculations of the linear and second-order nonlinear electric susceptibility tensor components of organic crystals. The methodology used for this purpose is based on a combination of the electrostatic interaction scheme developed by Hurst and Munn (Hurst & Munn, 1986) with electronic structure calculations for the isolated molecules. Our modification of the method consists in i) running periodic boundary condition (PBC) calculations for an adequate chromophore geometry (either experimental or optimized) to obtain atomic charges and in ii) performing the calculations of the molecular properties within a non-uniform embedding field generated by point charges located spherically around the reference molecule. Using this approach good accuracy is achieved on the electric susceptibility tensor components in comparison with the uniform dipole electric field (Seidler et al., 2013). We extend here the application of this method to other molecular crystals as well as we present the first attempt to predict the chi(1) and chi(2) components of two-component organic crystals (Gryl et al., 2014).

[1] *M. Hurst and R. W. Munn, J. Mol. Electron, 2, 35 (1986),* ***[2]*** *T. Seidler, K. Stadnicka and B. Champagne, J. Chem. Phys., 139, 114105 (2013),* ***[3]*** *M. Gryl, T. Seidler, K. Stadnicka, I. Matulková, I. Němec, N. Tesařová, P. Němec, CrystEngComm, doi:10.1039/C4CE00178H (2014).*

Keywords: linear and nonlinear optical properties, electrostatic interaction scheme, molecular crystals