**Monte-Carlo Simulation of the Incommensurate Structure of 4,4'-Diethoxyazoxybenzene**

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The aim of this work is to describe the behavior of an incommensurate molecular crystal using molecular dynamics simulations (MD). Incommensurate crystals are part of the more general class of aperiodic material. In addition to diffraction methods, molecular dynamical methods can be applied in order to give some information on the mechanisms leading to the aperiodicity of crystalline structures. Incommensurate crystals exhibit sometimes characteristics of disorder which should also be included in the modelling. The calculations are performed with the parallel code *ddgmq* [1]. The compound is 4,4 -diethoxyazoxybenzene (PAP) [2]. This compound exhibits two distinct crystalline phases from melting down to 100K. Phase II, stable above 356 K is described by a triclinic space group. Phase I is incommensurately modulated. The disorder is due to the distribution of the oxygen of the azoxy group on two possible sites.

Currently a model has been investigated in order to determine the correct sequence of the oxygen position with the development of a code based on the metropolis algorithm. Our aim is to find the configuration with the lowest energy. This structure will be used to initiate the molecular dynamic simulations.

[1] Brown D., Minoux H., Maigret B., *Comp. Phys. Comm.*, 1997, **103**, 170-186. [2] Pinheiro C.B., Gardon M., Pattison P., Chapuis G., *Ferroelectrics*, 2004, **305**, 83-87.

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