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Symmetry breaking and short-range order in aperiodic urea inclusion crystals

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Abstract

Here we will focus on the phase transitions and disorder within a prototype family of aperiodic compound n-alkane ($n\text{-C}_n\text{H}_{2n+2}/\text{urea}$), n varying from 7 (n-heptane) to 24 (n-tetracosane). A very rich sequence of phases is reported. All these phase transitions are described in terms of group/sub-group symmetry breaking within crystallographic superspace. Such phase transitions may either keep, decrease or increase the dimension of the crystallographic superspace. This result shows the multiplicity of structural solutions that aperiodicity offers. For short-chain guest molecules (from octane to dodecane), diffuse scattering is present in the form of sharp 2D-layers, depicting paracrystal features. The strong modulation of diffuse scattering within these layers shows that the positions of alkane molecules in neighbouring channels are correlated. Using the 3D- Δ PDF method, we have extracted the effective interaction potentials and have shown that the interaction is mediated by the relaxation of urea molecules.

References

A.Simonov, P.Rabiller, C.Mariette, L.Guérin, A.Bosak, A.Popov, and B.Toudic, Phys. Rev. B, in press.

(hk01) diffuse layer in n-octane-urea (exp & calc)

