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Diffuse scattering and phase transitions in aperiodic inclusion compounds

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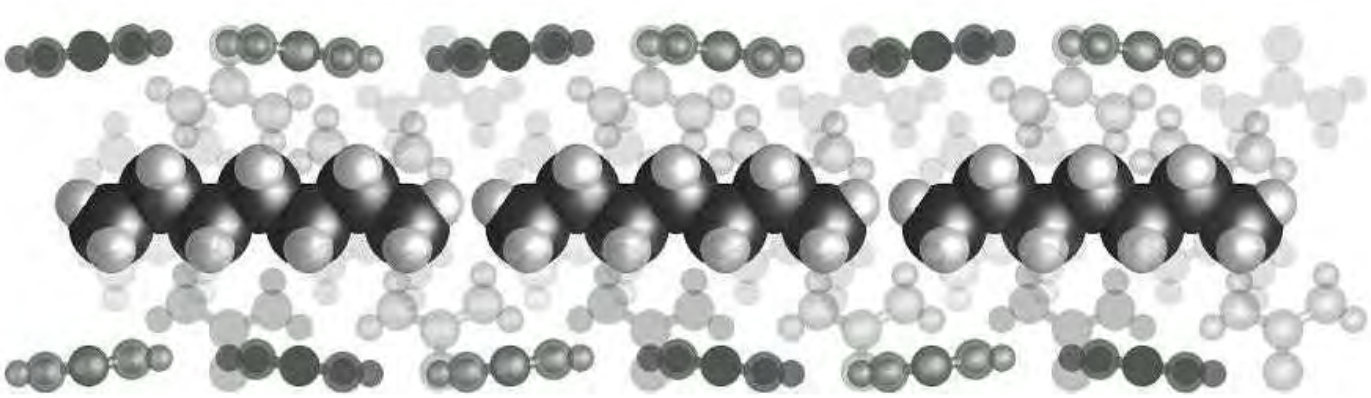
Small molecules, such as urea, thiourea, perhydrotriphenylene can be co-crystallised with long-chain hydrocarbon molecules to form inclusion compounds. The guest chains are confined to narrow, approximately cylindrical, channels created by the host small-molecule lattice. The stoichiometry and the conformations of the chains included inside the channels are function of internal interactions such as intra-chain interaction, but also of overall co-operative properties of the resulting three dimensionally ordered single crystal. These intergrowth compounds may form incommensurate composite crystals. A prototype example of such uniaxial intergrowth aperiodic crystals is n-alkane (CnH2n+2)/urea (CO(NH2)2). In these supra-molecular systems, urea molecules are connected by H-bonds and form helical ribbons, which repeat every six urea molecules to form a series of linear, hexagonal tunnels that can accommodate linear alkanes. Because the channels (~0.53 nm) are larger than the hydrocarbon chains, guests are held loosely and can undergo substantial motions. A significant amount of diffuse scattering of the first and second kinds can be depicted in scattering experiments, static or dynamic. These materials undergo a large variety of continuous or weakly first order structural phase transitions when changing the alkane molecule length and giving place to large pre-transitional effects. The talk will give an overview of the diffuse scattering in these compounds and will focus on connection with aperiodicity.



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