MS31 Unconventional interactions or symmetries for optimized and new properties, including chirality

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Simulation of lattice defects in quinacridone
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Abstract
Various lattice defects in the alpha-I-phase of quinacridone (C20H12N2O2) were simulated using lattice-energy minimisations. alpha-I-Quinacridone forms a chain structure in P -1, Z = 1. The molecules are connected by hydrogen bonds along [010], by pi-stacking along [100] and by weak van der Waals interactions along [001]. alpha-I-Quinacridone is inherently nanocrystalline. Lattice defects were calculated in correspondingly large supercells with up to 4464 atoms, using a previously evaluated force-field. Vacancies, vacancy aggregates and interstitial molecules are energetically very unfavourable. A misorientation of a single molecule (flip around [010] by 180°) causes an energy increase of 243.7 kJ/mol. Various edge defects and screw defects were investigated. A screw defect along [010] leads to E = + 76.1 kJ/mol, all other defects cause even greater energy increases. In contrast, the rotation of an entire chain around [010] by 180° leads to a very small energy increase only (E = 1.57 kJ/mol), and the real crystals probably contain a high number of such defects. Various planar defects were calculated, including different stacking disorders, anti-phase domains and commensurately modulated structures with two different types of layers having different lateral periodicities. Stackings faults along [001] with herringbone packing instead of parallel packing are energetically quite favourable; the same is true for antiphase domains in the [001] direction. As an example for a bulk defect we calculated antiphase domains, in which blocks of 4*4 chains are rotated by 180° around [010], which increases the energy only very slightly. Twinning by mirroring at the (001) plane is energetically favourable, and was observed in an HRTEM image. A rotation of chains, layers or block around [010] by 180° causes only a very slight modification of the molecular packing, which was not observable in the HRTEM. These investigations of lattice defects in alpha-I-quinacridone provide an insight to lattice defects, their energies and local structures in other similar organic chain structures, too.

References
D. Brey, B. Scherer, M.U. Schmidt, submitted.