



КАТЕДРА МЕТЕОРОЛОГИЯ И ГЕОФИЗИКА
ФИЗИЧЕСКИ ФАКУЛТЕТ - СУ "Св. Кл. Охридски"

Лавлокови четения :: Семинар „Кръстанов“

В петък, 12.07.2019 от 10:00 ч., в зала А209 на ФзФ - СУ

Проф. д-р Петър Векилов от Университета в Хюстън

ще изнесе (на български език) лекция на тема:

Olanzapine crystal symmetry originates in preformed centrosymmetric solute dimers

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Резюме: The symmetry of crystals is a central quality that determines their function and allure. Given the uncorrelated symmetries of a crystal and its constituent molecules, the symmetry breaking that begets a crystal phase has been thought to ensue during nucleation. Here we demonstrate that the one of the two symmetry element of olanzapine crystals, an inversion center, emerges in solute dimers extant in the solution prior to crystallization. Time-resolved in situ atomic force microscopy shows that crystals grow nonclassically, exclusively by incorporation of dimers; this growth mode has been speculated and inferred from crystal and solute structures, but never experimentally observed. The growth rate of crystal layers exhibits a quadratic dependence on the solute concentration, characteristic of the second-order kinetics of dimer incorporation. The free energy of dimerization of olanzapine from all-atom molecular dynamic (MD) simulations support the experimental observation that olanzapine dimers constitute a minority solution component. We also show that growth by dimers is preferred not owing to greater activation entropy or faster dissociation of attached solvent molecules. The adsorption free energies of dimers and monomers on the olanzapine crystal surface from MD simulations suggest preferential adsorption of the dimer on the surface that results in overwhelming accumulation of adsorbed dimers and expedites their incorporation into growth sites. The proposed outlook on the cooperative creation of crystal symmetry illuminates analyses of structure selection, polymorph transformations, chiral separation, and crystal properties of natural and engineered crystals.

Всички заинтересовани са добре дошли!