The effect of urea additives on the physicochemical characteristics of crystals

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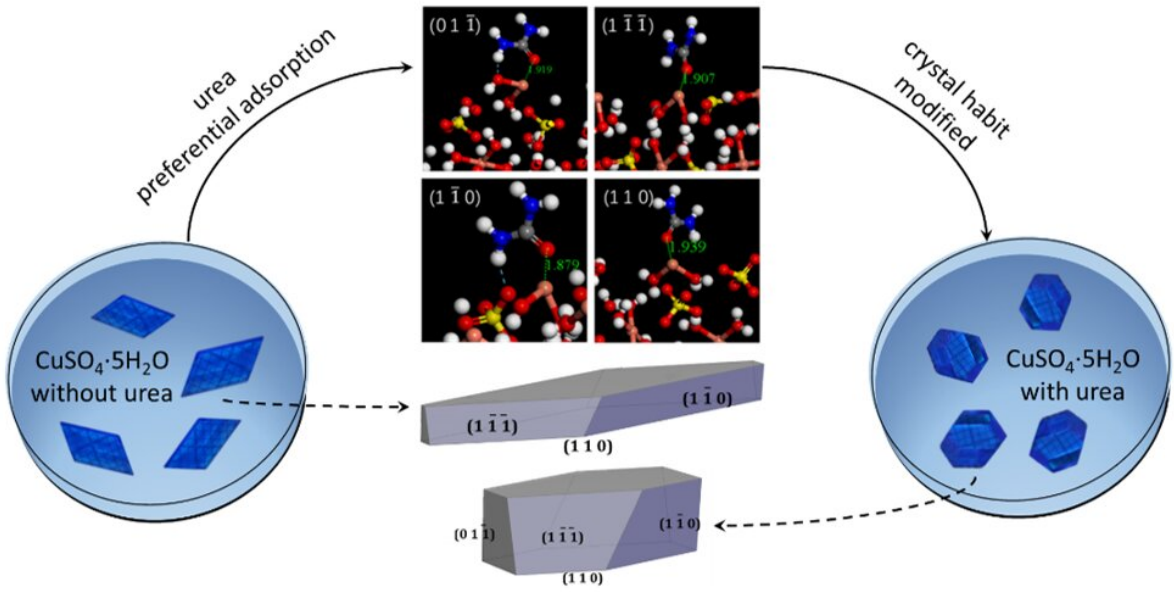

Schematic illustration of the effect of urea additive on $CuSO_4 \cdot 5H_2O$ crystal habit. Credit: Prof. ZHUANG's group)

Crystal habit has a considerable impact on the physicochemical characteristics of crystals, and understanding that is meaningful for the control of functionality in modern materials and chemical industry.

In a study published in *CrystEngComm*,a research team led by Prof. Zhuang Xinxin from Fujian Institute of Research on the Structure of

Matter (FJIRSM) of the Chinese Academy of Sciences revealed the effect of urea additive on $CuSO_4 \cdot 5H_2O$ crystal habit.

The researchers found that $CuSO_4 \cdot 5H_2O$ forms an oblique hexagonal prismatic, which is distinct from the naturally grown parallelogram. They showed that the growth rates of (0 1 -1), (1 -1 -1), (1 -1 0) and (1 1 0) faces of $CuSO_4 \cdot 5H_2O$ depend strongly on urea concentration, and the additive has two opposite effects that can be attributed to the combined impacts of thermodynamic factor and kinetic factor.

To rationalize the mechanism from a molecular perspective, the researchers obtained the geometries and the adsorption energies of water and urea molecule on specific faces utilizing density functional theory (DFT) calculations. The DFT calculation results indicated that the formation of H_2O-Cu bond was hampered by the binding of carbonyl group (C=O) of urea to the Cu atoms, and the significant distinction of the adsorption energies proves the preferential adsorption of urea on (0 1 -1) face.

Few studies have been carried out in this regard as the unit cell structure of $CuSO_4 \cdot 5H_2O$ is more sophisticated and may show greater variety in the process of adsorption than the existing studies. This study comes up with a new approach in the $CuSO_4 \cdot 5H_2O$ crystal habit modification, explains the mechanism from a molecular perspective rationally, and is instrumental for evaluating the organic additives with specific functional groups under the guidance of theoretical calculations.

More information: Shigui Zheng et al. Effect of urea additive on CuSO4·5H2O crystal habit: An experimental and theoretical study, *CrystEngComm* (2020). DOI: 10.1039/D0CE00115E

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