

'CrystEngComm' cover story features S&T research

Posted by Kimber Crull On May 2, 2023

Dr. Rainer Glaser, interim vice provost for graduate education and professor of chemistry, and Harmeet Bhoday, a Ph.D. student in chemistry, recently published an article in CrystEngComm titled "Polar and non-polar stacking of perfectly aligned parallel beloamphiphile monolayers (PBAMs) of (PhO, F)-azine. The interplay of non-covalent interlayer interactions and unit cell polarity." The article was highlighted on the cover of the April 2023 issue.

The central question of the present paper concerns the origin of the difference in the stacking of the parallel beloamphiphile monolayers (PBAMs) in the antiferroelectric and ferroelectric polymorphs I and II of (PhO, F)-azine. Both polymorphs feature identical 2-D PBAMs that stack in polar and nonpolar fashion in the third dimension, this kind of polymorphism is unprecedented and unexpected. It is the interlayer binding between the PBAM surfaces that decide the final crystal architecture, polar or non-polar stacking. In the case of (PhO, F)-azine both stacking options are realized because both options are associated with interlayer binding of comparable strengths. The antiparallel stacking offers a small but significant advantage for the interlayer binding of the PBAMs.



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