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**Monday, 15 April 2024**

**4:00 pm in 303 Schrenk Hall**

***Polar and Non-Polar Stacking of Perfectly Aligned Parallel Beloamphiphile Monolayers (PBAMs) in Organic Molecular Crystals by Rational Design: The Interplay of Non-Covalent Intermolecular Interactions***

**Abstract:** Polar donor-acceptor substituted organic molecular crystals are promising for their wide range of applications in the realm of non-linear optics (NLO), ferroelectricity, and fluorescence. However, the achievement of dipole parallel-alignment in organic donor-acceptor substituted molecular crystals has been challenging as most polar molecules crystallize in a way as to compensate for the dipole moments producing a non-polar crystal. It was believed for a long time that achieving any polar order is almost impossible as the electrostatic repulsions related to parallel alignment are invincible. However, our studies have shown that the rational design of polar molecular crystals is feasible. Following our rational design strategy, we have been able to grow polar crystals for a variety of donor(X)-acceptor(Y) acetophenone azines (C=N–N=C spacer group), which we refer to as (X, Y)-azines. Perfect polar order throughout the parallel beloamphiphile monolayers (PBAMs) has been achieved first with the X = methoxy series (Y = Cl, Br, I) and recently with the X = phenoxy series (Y = F, Cl, Br, I). Perfect polar stacking was achieved for (PhO, Y)-azines with Y = Cl, Br, I. The case of (PhO, F)-azine is a special one as we were able to grow two polymorphs, **I** and **II**. The striking contrast between the polymorphs is the stacking of the PBAMs in the third dimension. The difference in stacking demonstrates the subtle role of weak non-covalent interlayer interactions and unit cell polarity in affecting the crystal architecture.