

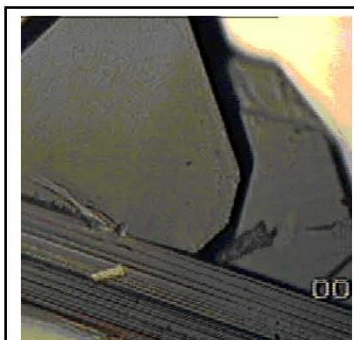
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Controlling and Understanding Emergent Behavior in Molecule-based Materials

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The manners in which molecules arrange themselves in the solid state have significant implications for their electronic and magnetic properties. Small energy differences between polymorphic structures can enable crystallization conditions to dictate the phase of the crystallized product. In many cases, competition for directional intermolecular interactions, including hydrogen and halogen bonds, enables stimuli-responsive behavior, including pressure-induced phase transitions. This talk provides an overview of the assembly of molecular components in conductive cation radical salts and magnetic coordination polymers, including the selective crystallization of various polymorphs. For cation radical salts, five polymorphic phases in the $(\text{BEDT-TTF})_2\text{Ag}(\text{CF}_3)_4$ (1,1,2-trichloroethane) system have been crystallized, four of which have superconducting ground states. In this case, phase selectivity is enabled by the current density during the electrocrystallization process. Among the superconducting salts, the ones with intercalated charge ordered layers exhibit a five-fold enhancement of T_c . We also show that pressure can be used to selectively crystallize magnetic coordination polymers. This will be illustrated for both solid-state and solution-based methods. Furthermore, post-synthetic application of pressure provides a means to control electronic and magnetic coupling. For example, pressure-induced sequential reorientation of the Jahn-Teller axis in $\text{CuF}_2(\text{H}_2\text{O})_2(\text{pyrazine})$ results in a change in magnetic dimensionality with higher pressure leading to a chemical transformation. Future directions and opportunities for molecule-based electronic/magnetic materials will be discussed.



Preferential growth of the kinetic and thermodynamic superconducting phases of $(\text{ET})_2\text{Ag}(\text{CF}_3)_4(\text{TCE})$ can be controlled by current density.

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