Polymorphism of Lanthanoid (III) Diphthaocayanines as Qubit Candidates

Maegan Dailey | Graduate Student, Besson Lab, Department of Chemistry

Lanthanoid (III) diphthaocyanine (LnPc$_2$) complexes have attracted significant interest in the past due to their interesting magnetic properties. The large anisotropy of the lanthanoid centers makes these complexes good candidates for single-molecule magnets, which in turn are part of the reason why these complexes are potential quantum bits, or qubits. Why are we interested in molecules that act as single molecule magnets and are potential quantum bits? So we can build a quantum computer, which has many applications such as encryption. However, it is not only the lanthanoid centers that make these complexes so interesting. The aromatic phthalocyanine ligands enhance access to the magnetically competent f-orbitals on the lanthanoid centers. Additionally, these ligands can be modified to assess the impact of electronic and steric factors on the magnetic properties. Presented here is a comparison between the synthesis and characterization of unsubstituted LnPc$_2$ and halogenated LnPc$_2$ complexes, the latter of which have been unexplored thus far. A one-pot reaction followed by purification with size-exclusion chromatography has proven to be a reliable method that leads to a variety of crystalline polymorphs, which have been investigated by X-ray crystallography. Presented here is also a comparison of single-crystal conductivity measurements on these various polymorphs. By studying both substituted and unsubstituted LnPc$_2$ complexes, a better understanding can be obtained of how various factors, such as oxidation state and crystal structure, impact magnetic relaxation. Understanding what impacts magnetic relaxation is an important and necessary step in building better qubits.

Softening of Rapidly Heated Nanoscale Glassy Films of Methylbenzene

Rinipal Kaur | Graduate Student, Sadchenko Lab, Department of Chemistry

Using Fast Scanning Calorimetry, we investigated the impact of thin film confinement on softening and vaporization of glassy films of methylbenzene in the limit of high heating rates. The glassy films of distinct thicknesses ranging from 2 to 1800 nm were grown by vapor deposition and subjected to heating with rates in excess of 100 kilo-K/s. For the films with thicknesses above 20 nm, the resulting softening kinetics strongly implied a surface facilitated mechanism: the softening originated at surfaces of a sample and progresses into its bulk via a transformation front. Yet, according to our analysis, the kinetic parameters for the softening front propagation differed significantly for films with thicknesses below and above 300 nm. For example, the apparent activation energy barrier for the front propagation almost doubled for thicker films. We interpret these results in the framework modified Wilson-Frenkel model of softening front propagation and discuss their implications for past FSC studies of nanoscale vapor-deposited glassy films.

Friday, November 16, 2018
SEH B1220 2:00-3:00 p.m.
Refreshments will be served at 1:45 p.m.