

# PHYSICAL CHEMISTRY SEMINAR



**Prof. Lisa Fredin**

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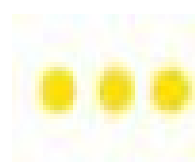
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Monday, November 13, 2023

4:00 PM | YH 4222

Mani L. Bhaumik Collaboratory -  
Dongwon Yoo Seminar & Conference Hall

## Modeling Photoactive Organic Materials



**Abstract:** Chemical intuition is well developed for single molecules but the extent to which disorder in solid state molecular materials contributes to their properties is poorly understood. In particular, molecular materials move charges in some directions much more efficiently than others due to the packing of the molecules. Noncovalent interactions between the molecular components mean that dynamic disorder in these materials can have a large impact on the electronic properties of these materials at room temperature. This work explores how packing and vibrations in organic crystals affect charge transport in light driven devices. In particular, the size of dynamic disorder due to phonons or electronic excitation of molecules in the crystal is predicted for well-ordered high-mobility single crystals.