

## Chem 218: Student Exit Seminar

# “Tuning the Excitonic Properties of 2-Dimensional Molecular Aggregates across the Visible and Shortwave Infrared”

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Molecular aggregates are non-covalent self-assemblies of chromophores wherein transition dipole moments of individual molecules couple coherently over long distances, forming delocalized excitons. This imparts exciting photophysical properties such as extreme blue or red shifts (seen in H- or J-aggregates respectively), narrow linewidths and high molar absorptivities. We modulate the transition dipole couplings within an aggregate via molecular packing, topology, and disorder in order to tune and explore new photophysical behaviors. In this talk, I will discuss the unusual situation that arises from 2D transition dipole coupling in sheet-like aggregates. In addition to traditional H- and J-aggregation, we find a new case of ‘*I-aggregation*’ which shows intermediate characteristics of H- and J-aggregates. I will also describe how we use thermodynamics of self-assembly to control the aggregate packing and thereby, tune excitonic properties. Using a three-component equilibrium model, I will lay down general principles for selectively stabilizing H- or J-aggregates, allowing us to construct a library of 2D J-aggregates with absorptions spanning the visible and shortwave infrared (SWIR) regions. Finally, I will show how subtle differences in chromophore structures within this library modulate the aggregate packing and eventually lead to distinct excitonic band pictures, that can be experimentally probed using temperature dependent spectroscopy. Overall, this work establishes molecular aggregation as a tunable avenue for accessing unusual photophysical properties and thus, opens up organic chromophores to new functionalities including SWIR imaging, plexitonics, and telecommunications.



Thursday, February 11<sup>th</sup>, 2021  
12:00 p.m. (PST)