Subsystem Quantum Chemistry for Molecular Materials

A talk by Christoph R. Jacob

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Materials built from molecular building blocks provide a promising novel approach to materials with specific properties via chemical modifications of the molecular building blocks. Molecular materials play an important role in organic photovoltaics and could provide a new approach to designing metamaterials with a negative index of refraction.

In my talk, I will discuss the development of quantum-chemical tools for understanding and designing such materials. Subsystem quantum-chemical methods provide a natural route to connecting the properties of the molecular building blocks to the macroscopic properties of the molecular material.

First, I will discuss the identification of plasmonics excitations in the molecular building blocks. Second, the embedding of the molecular building blocks with subsystem density-functional theory will be considered. Finally, approaches for including the coupling between the molecular building blocks will also be introduced.