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LEHIGH UNIVERSITY | Institute for Functional Materials and Devices (I-FMD)

What our lab does:

- Builds computational models of experimental materials, including defects, surfaces, and disorder.
- Uses quantum mechanics and other electronic structure theories to build better understanding of structure-property relationships for complex materials.

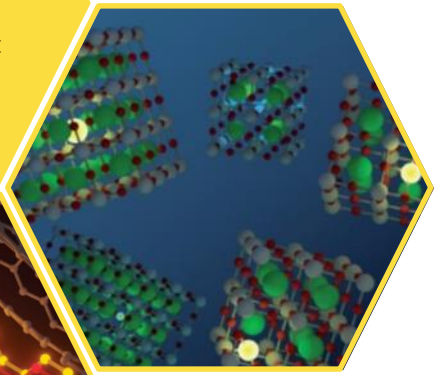
Our Models:

- Combine molecular and material descriptions.
- Bridge physical chemistry, material science, nanoscience, and computation.
- Probe the boundaries of the particle and wave approximations of electrons in materials.

Why we are investigating this area:

- Organic materials are flexible, low cost, and tunable.
- Inorganic oxides are highly reactive for photocatalytic conversion of water or carbon dioxide.
- With better understanding of the photophysics and reactivity of materials → we can *rationally design materials* with *targeted properties*.

We model both **inorganic** metal oxide materials and nanocrystals, as well as **organic** molecules and materials.



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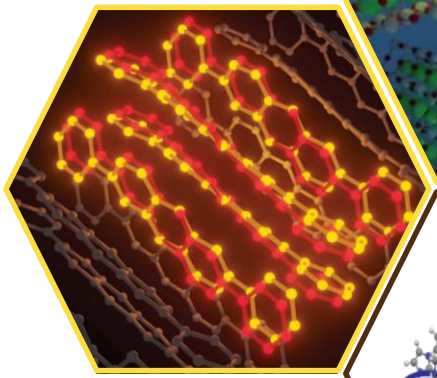

10.1021/acs.jpca.2c02120