Designing Electronic Properties of Metal-Organic Chalcogenides

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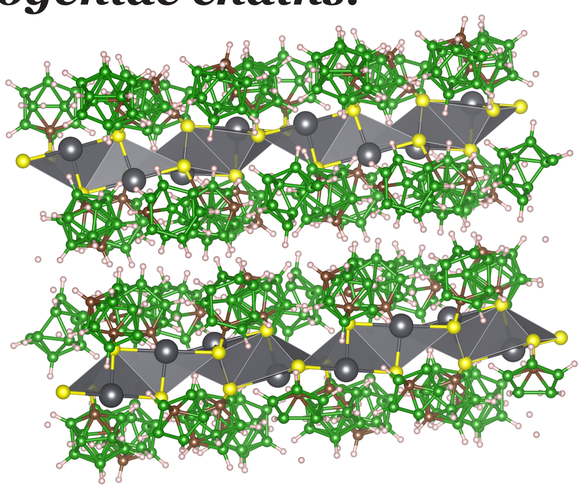
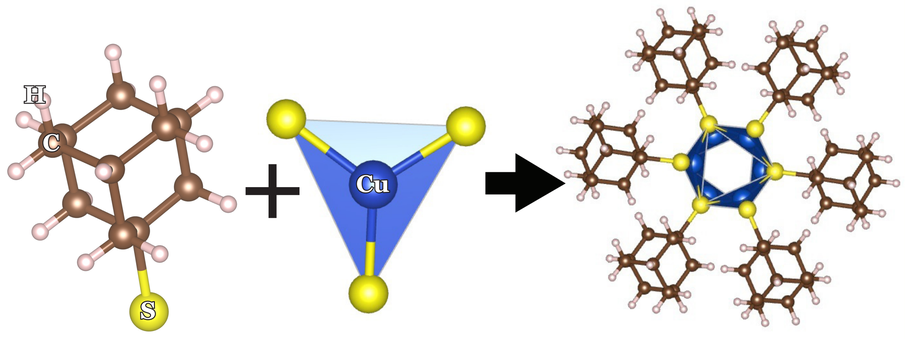
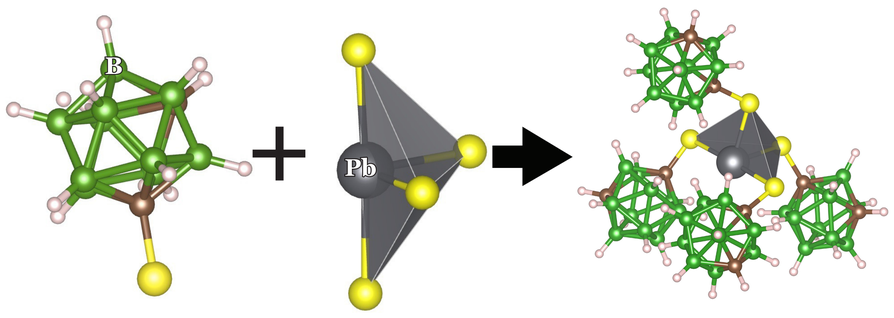
With metal-organic chalcogenides, we can harness the variety of geometry of organic molecules to tune the electronic properties of chalcogenide chains.

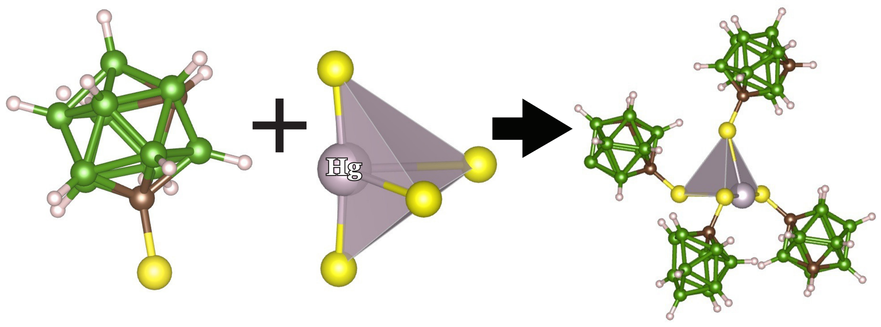


Changing ligands and inorganic composition can yield diverse crystal geometries...





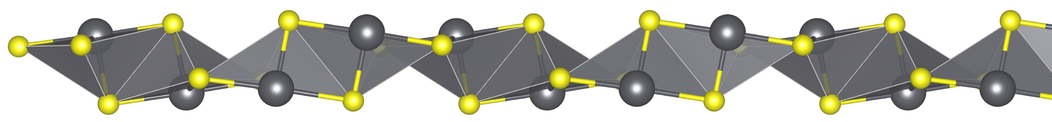
...or variations of similar structures.



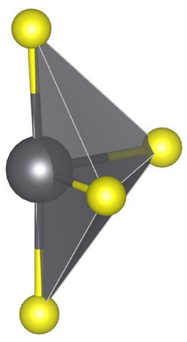
If we can tune the inorganic structure by changing the ligand or inorganic composition, what geometric changes yield the most interesting electronic properties?

To understand the impact of crystal geometry on electronic interactions, we study continuous deformations of crystal structures.

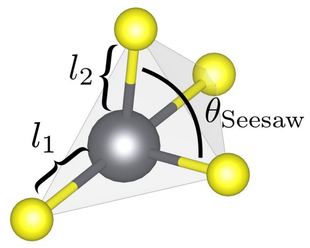
OUR METHOD



1. Develop a parametric model from existing or new structures.

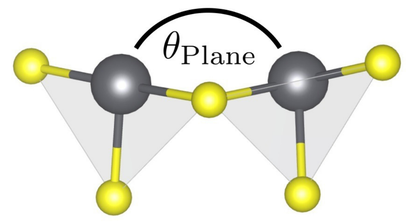


Identify the building unit(s).

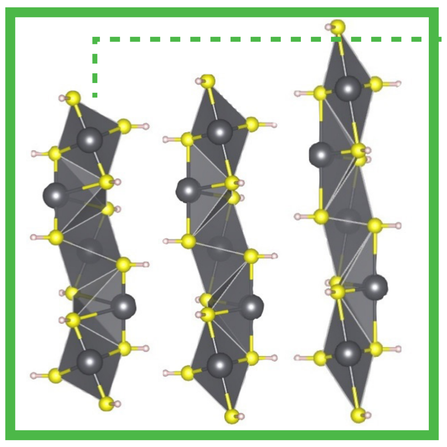


Parameterize unit(s).

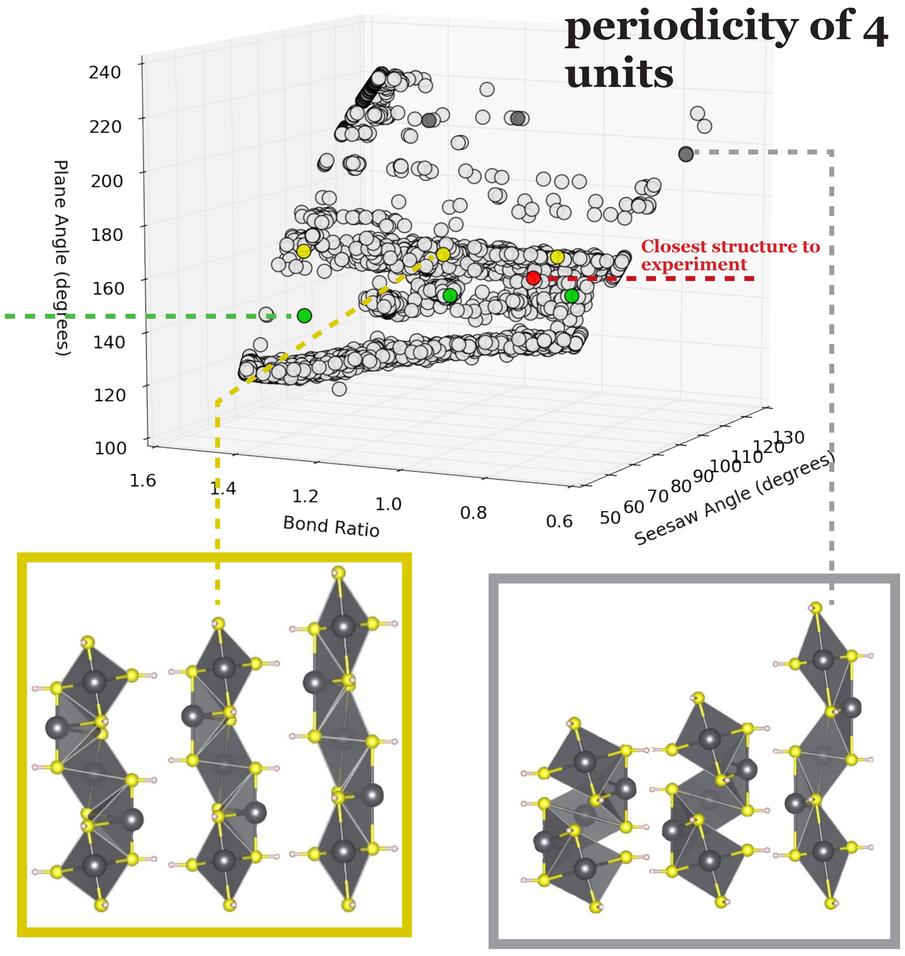
Parameterize geometric relation between units.



2. Optimize continuous parametric model for periodic calculations.

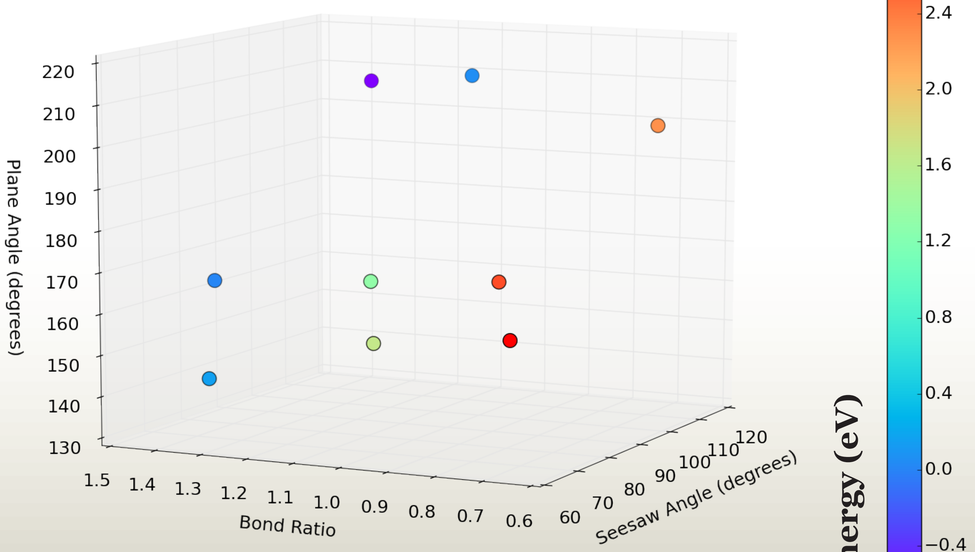


Structures with periodicity of 4 units



3. Use low-level density functional theory to extract basic electronic properties.

Indirect Band Gap of Select Structures



4. Correlate properties to changes in geometry to find desirable structures.

(5.) Find ligands that support desirable structures.

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