Using Quantum Simulations to Analyze Electron Behavior in Tetrahedrally Bonded Materials

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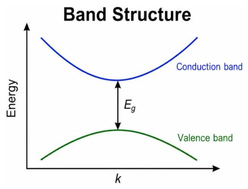
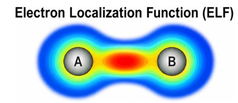
Background



- The electronic energies in the k-space.



- A real-space map of electron localization. derived from Pauli exclusion.

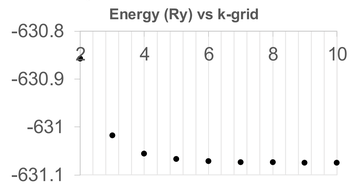
Research Question

How does the band structure and electron localization change in tetrahedrally bonded materials as they transition from having insulative to conductive properties?

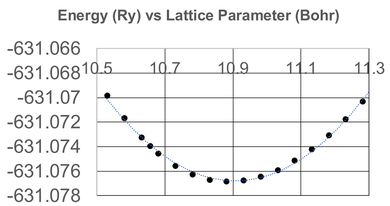
Fig. 1. Isolated tetrahedral bonding.

Methods (Quantum ESPRESSO)

- Quantum ESPRESSO is a computer program that simulates material properties by using Density Functional Theory (DFT).
- Before analyzing electronic structure and ELF, key computational parameters were converged to balance numerical accuracy and computational efficiency.



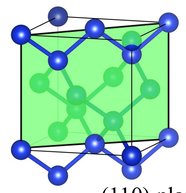
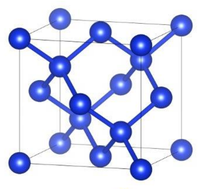
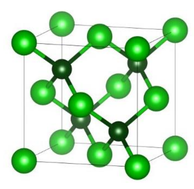
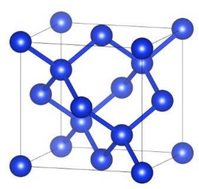
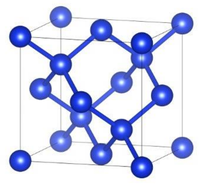
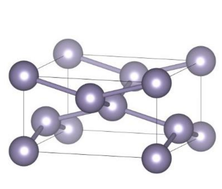
A) *k*-point Convergence



B) Lattice Parameter Optimization

Fig. 2. Optimizations for germanium.

Materials

Diamond (Carbon)	Silicon	Gallium Arsenide	Germanium	α-Tin	β-Tin
 (110) plane					
Insulator	Semiconductor	Semiconductor	Semiconductor	Semimetal	Metal
Indirect band gap	Indirect band gap	Direct band gap	Indirect band gap	Zero band gap	No band gap

Results

Band Structures

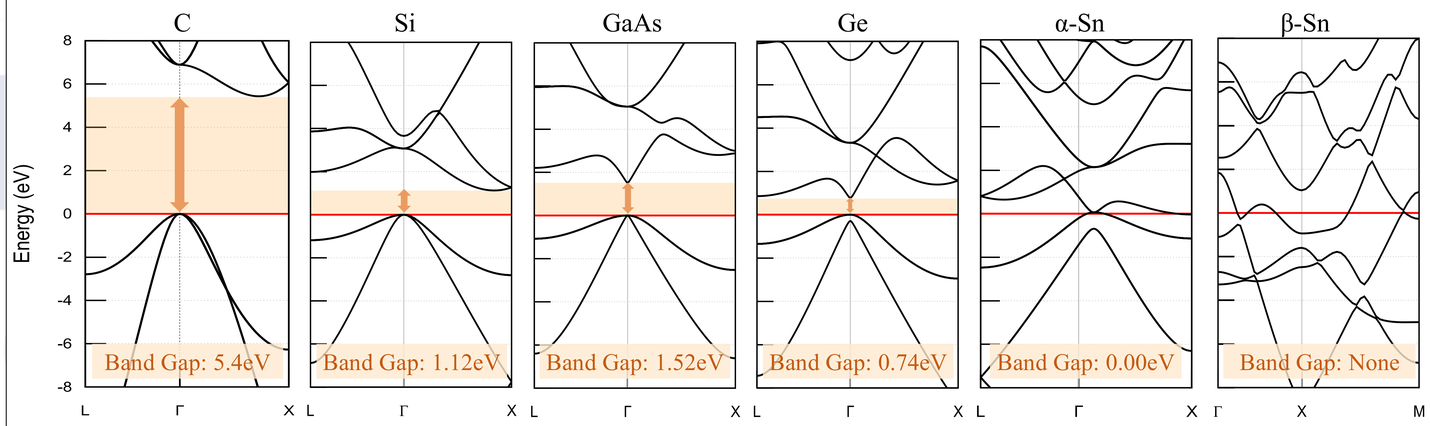


Fig. 3. Band structures show electron energies versus crystal momentum. Smaller band gaps indicate more metallic behavior. Orange boxes mark the band gaps.

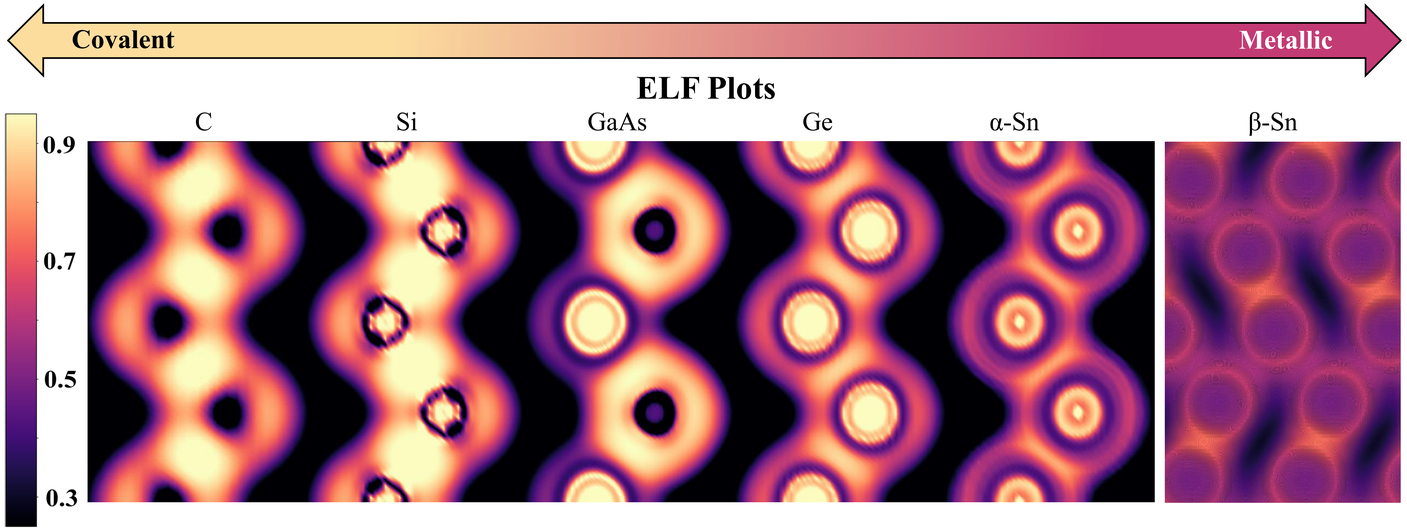


Fig. 4. ELF on the (110) plane: high ELF = localized electrons; ELF ≈ 0.5 = delocalized behavior. Core/nucleus colors are software artifacts.

Discussion

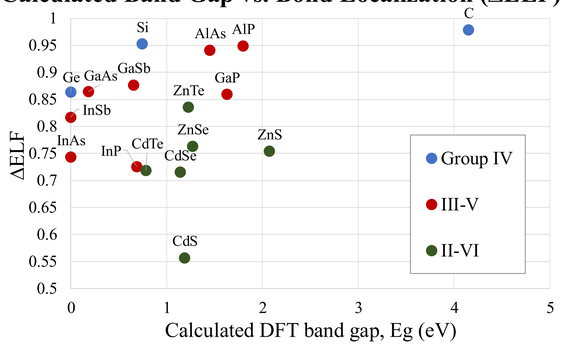
- Quantum ESPRESSO typically underestimates semiconductor band gaps and overestimates lattice parameters.

% error	C	Si	Ge	GaAs	α-Sn
Δa (%)	1.78	0.6823	1.121	1.782	3.4
ΔE_g (%)	-24	-36.6	-100.0	-87.1	N/A

ΔELF vs Band Gap (E_g)

- ΔELF measures the largest ELF at the center of the bond compared to a non-bonding region.
- Results suggest a qualitative link between real-space bonding and reciprocal-space energetic levels.

Calculated Band Gap vs. Bond Localization (ΔELF)



Emerging Research Questions

- Investigate whether ELF correlates with mechanical properties such as brittleness.
- Investigate how to account for bond ionicity to more strongly correlate ΔELF and E_g.

Conclusion

- Electrons are delocalized and free to move when the valence and conduction bands overlap. Conversely, electrons are "trapped" within bonds when a band gap is present.
- Across tetrahedrally bonded materials, electron localization decreases as a material's metallic character increases.
- Quantum ESPRESSO successfully reproduced electronic structures and properties
- A loose link is suggested between ELF in real space and band gaps in reciprocal space

References

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