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Center for Computational Quantum Physics

Exploring Super Atomic Crystals

NSBP Innovate Seminar Series

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About Me

- Studied classical ballet and modern dance for 10 years
  - Earned B.A. in dance from New School University
- Transitioned to STEM
  - Earning B.S. in physics at Brooklyn College at CUNY
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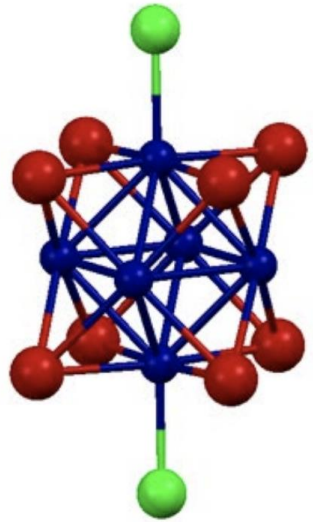
Topics

- What is a super atomic crystal?
- How do we use computational materials science techniques to discover their properties?
- How can these properties potentially improve certain technologies?

What is a Super Atomic Crystal?

Super Atoms

- **Super atoms** are stable discrete clusters of atoms
- Mimics properties of traditional atoms
- Complex structure allows tuning for their magnetic, electrochemical, and photonic properties



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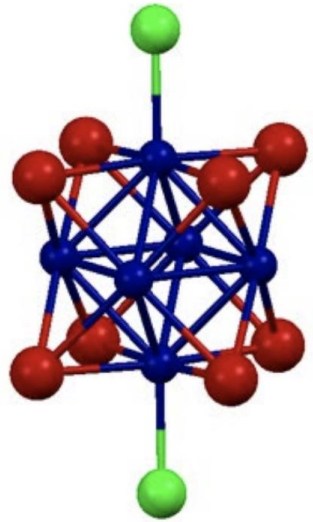
Super Atoms

- Sized between molecules and bulk solids
- Typically have capping ligands that stabilizes cluster
- Directs self-assembly and control coupling between clusters
- Assembly leads to a highly delocalized electronic structure in their s-like, p-like, and d-like orbitals
- Includes metal chalcogenides, fullerenes, and aluminum clusters



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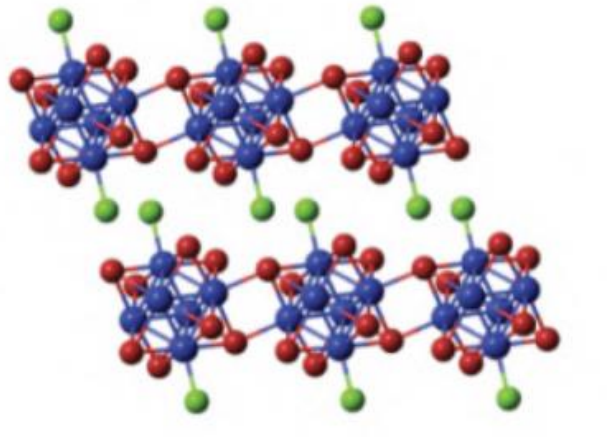
Super Atomic Crystals

- Super atoms bound together form **super atomic crystals**
- Coupling forms 2d and 3d bulk structures, each of which can offer slightly different properties
- Provides great opportunities in materials design such as nanoelectronics, energy generation and storage, and quantum computing



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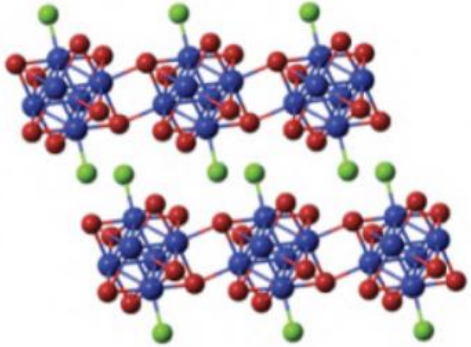
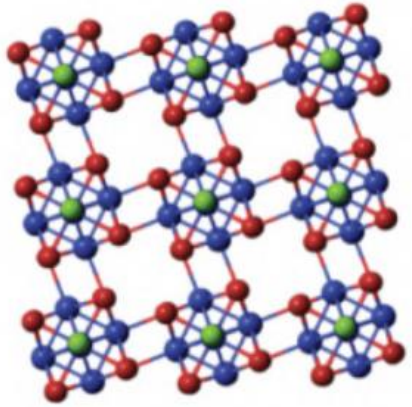
$Re_6Se_8Cl_2$

- Stacks of weakly interacting 2D sheets (left)
- Single 2D sheet on of strongly bonded super atomic clusters (right)
- Semiconductor at room temperature with wide electronic band gap
- Further study on its electronic structure needed



$Re_6Se_8Cl_2$ (side view) – two stacks of weakly interacting sheets



$Re_6Se_8Cl_2$ (top view) – 2D sheet of strongly bonded super atomic clusters

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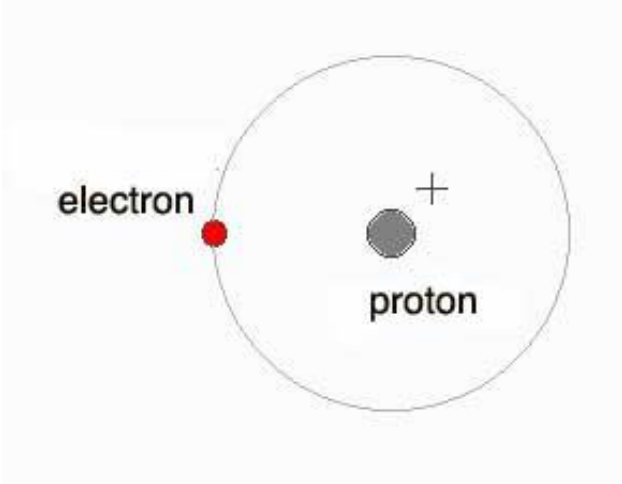
How do we used computational materials science techniques to discover their properties?

Schrödinger's equation

- Used to describe electronic structure
  - **Electronic structure** describes arrangement of electrons in an atom, molecule, or crystal structure
- Can be solved exactly for simple electronic structures
- Computationally impossible to solve exactly beyond simple structures

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)$$



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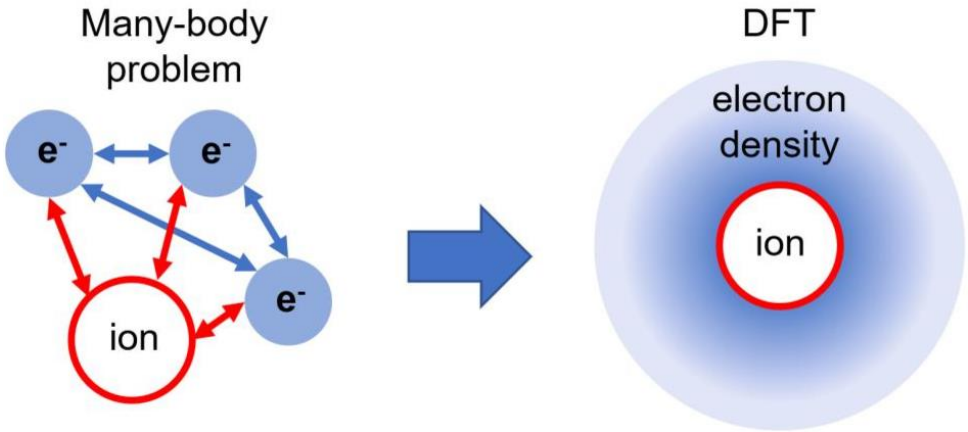
Density Functional Theory (DFT)

- Solves Schrödinger equation approximately for many-body quantum systems
- Also describes vibrations and electronic structure of atoms, molecules and solids
- Workhorse for computational materials science



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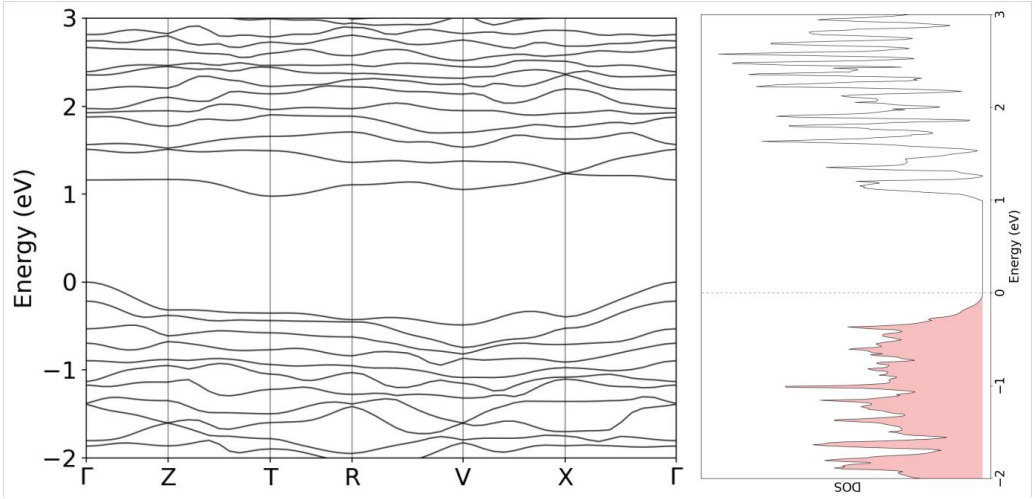
DFT Software Packages

- Many open-source packages available to perform electronic structure calculations
- Interest in quantum mechanics and intermediate level programming skills
- World-wide STEM community with a growing interest in software development within science

Band Structures

- Band structures show weak interactions between Kohn-Sham orbitals
- Indirect bandgap with valence band maximum at Γ point and conduction band minimum at T band
- Bandgap of 1. 1 eV confirms semiconducting properties



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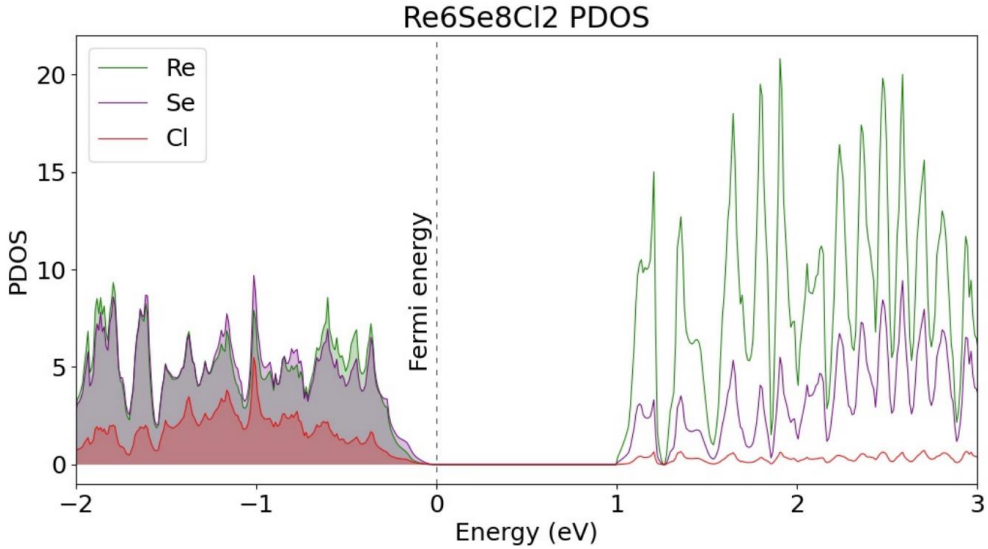
Total Projected Density of States

- Calculated projected density of states for Re, Se, and Cl orbital contributions
- Re and Se provides highest orbital contributions at valence bands
- Re provides highest orbital contribution at conduction bands



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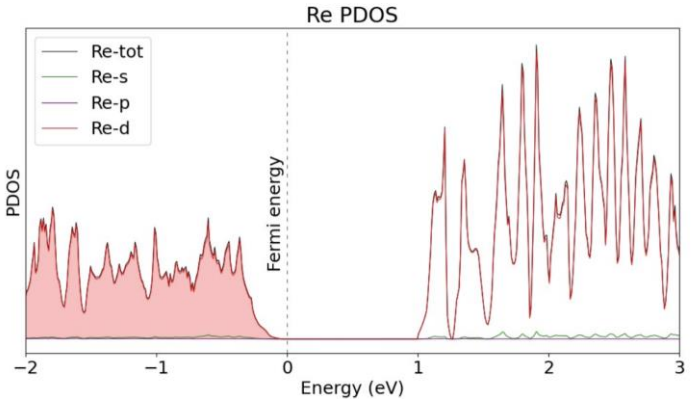
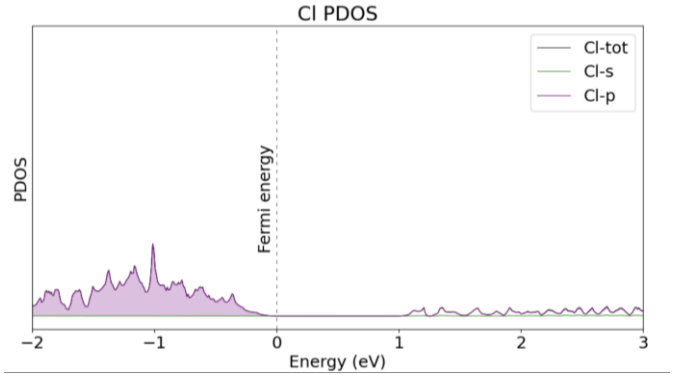
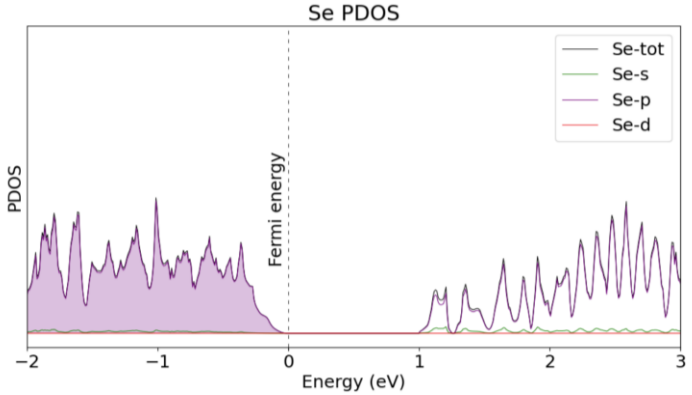
Atomic Orbital Projected Density of States

- Determines how each atomic orbital contributes to electronic structure
- Re d-orbitals and Se p-orbitals highest orbital contribution
- Re d-orbitals highest orbital contribution for conduction bands







How can these properties potentially improve certain technologies?

Semiconductors and Superconductors: Silicon

- Advantages
  - Second most abundant element
  - Indirect bandgap within the semiconductor range
  - Relatively low manufacturing cost
  - Safe handling of large wafers
  - Thermally stable up to 1100°C
- Disadvantages
  - Expensive to produce Si crystals
  - Short life cycle
  - Brittle
  - Produces environmentally harmful waste

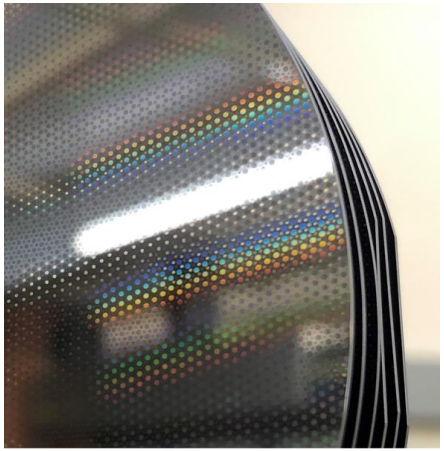
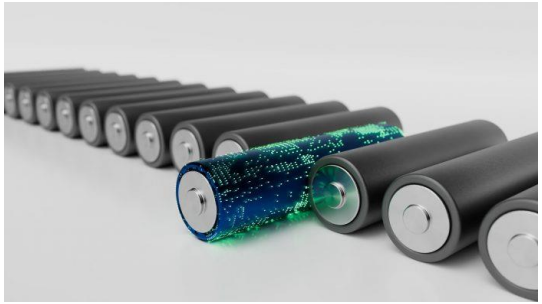


Photo of a stack of shiny silicon mirrors. The top one is coated with etching patterns featuring repeating small circles. Some are rainbow colored when catching the ambient light.

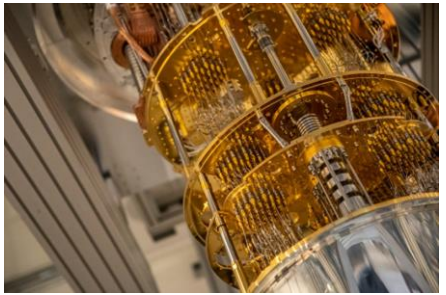
Properties of Super Atomic Crystals

- Complex structure allows for tunability
  - 2d layers can have a different band gap compared to 3d bulk solid
  - Doping shown to increase optical transport
  - Capping ligands and covalent bonds allow for stability
  - Could mean longer life cycle of material
- Can exhibit both semiconductor and superconductor properties
- Stable under ambient temperature

A row of solar cells underneath the shining sun which, in general, can convert ~24% of sunlight into electricity.



"(Lithium-ion battery technology) is focused on extending and expanding rapid-charge-discharge technology and battery life." – Innovation News Network



DOE's Lawrence Berkeley National Laboratory is using a sophisticated cooling system to keep qubits – the heart of quantum computers – cold enough for scientists to study them for future use in quantum computers.

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Summary

- Defined what a super atom and a super atomic crystal is
- Outlined the computational material science techniques used to study their electronic structure
- Shared the properties that could potentially improve certain technologies

Scan to learn more about my work, including research, software development, and speaking engagements

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Thank You!

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References

- Asim, N., Sopian, K., Ahmadi, S., Saeedfar, K., Alghoul, M. A., Saadatian, O., & Zaidi, S. H. (n.d.). *A review on the role of materials science in solar cells*. https://doi.org/10.1016/j.rser.2012.06.004
- Giannozzi, P., et al. (2009). Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 21(39).
- Giustino, F. (2014). Materials modelling using density functional theory : properties and predictions.
- Kokalj, A. (1999). XCrySDen-a new program for displaying crystalline structures and electron densities. Journal of Molecular Graphics and Modelling, 17(3–4), 176–179.
- Posysaev, S. (2018). Applications of density functional theory for modeling metal-semiconductor contacts, reaction pathways, and calculating oxidation states.
- *PV Cells 101: A Primer on the Solar Photovoltaic Cell | Department of Energy*. (n.d.). Retrieved November 28, 2022, from https://www.energy.gov/eere/solar/articles/pv-cells-101-primer-solar-photovoltaic-cell

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References

- Varma, A., Badam, R., James, A. L., Higashimine, K., Jasuja, K., & Matsumi, N. (2022). Titanium Diboride-Based Hierarchical Nanosheets as Anode Material for Li-Ion Batteries. *ACS Applied Nano Materials*. https://doi.org/10.1021/ACSANM.2C03054
- *What is hydrogen? Atoms and Chemistry - Quatr.us Study Guides*. (n.d.). Retrieved November 28, 2022, from https://quatr.us/chemistry/hydrogen-atoms-chemistry.htm
- Yang, J., Russell, et al. (2021). Superatomic solid solutions. Nature Chemistry, 13(6), 607–613.
- Zadrozny, J. M., Niklas, J., Poluektov, O. G., & Freedman, D. E. (2015). Millisecond coherence time in a tunable molecular electronic spin qubit. *ACS Central Science*, *1*(9), 488–492. https://doi.org/10.1021/ACSCENTSCI.5B00338
- Zhong, X., Lee, K., Choi, B., Meggiolaro, D., Liu, F., Nuckolls, C., Pasupathy, A., De Angelis, F., Batail, P., Roy, X., & Zhu, X. (2018). Superatomic Two-Dimensional Semiconductor. Nano Letters, 18(2), 1483–1488.
- Geometric optimization provided by Petra Shih of the Berkelbach Lab

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