Manipulation of Atomic Ordering for Manufacturing Semiconductors (µ-ATOMS)
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Mission Statement: *To discover the underlying science principles determining the ordering of atoms in semiconductor alloys.*

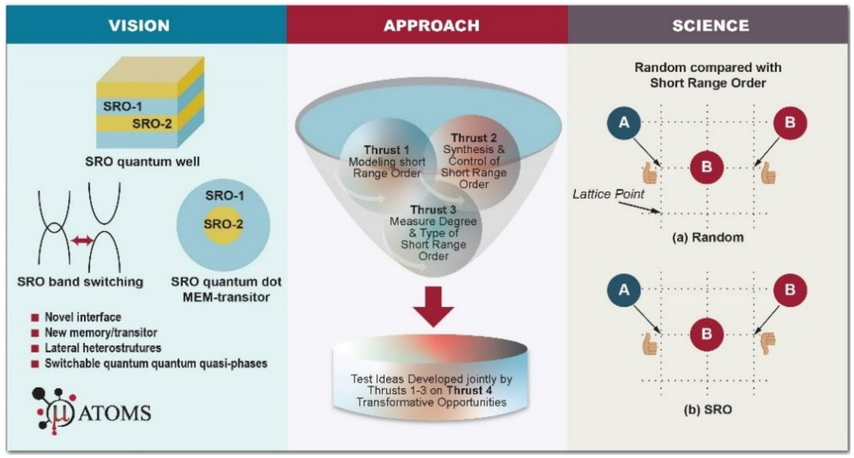

Figure 1 Vision: Precision manipulation of the spatial correlation among atoms as opposed to composition or dopants, to fabricate semiconductor properties using only one composition. **Approach:** Thrust 1-3 integrated into crosscutting Thrust 4 to demonstrate ability to design semiconductor properties and novel structures creating transformative opportunities. **Science:** SRO (a) Random – no restriction on nearest neighbors; (b) SRO - restriction on nearest neighbors.

The mission of the µ-ATOMS Energy Frontier Research Center is inspired by much of the work the research team recently uncovered on novel Group IV alloy semiconductor materials, demonstrating that short-range order (SRO) of Ge and Sn atoms on the periodic lattice of GeSn has a very large effect on the electronic energy band gap. SRO describes the probability that the nearest neighboring atoms to any B atom *(Figure 1)*, are restricted on average to NOT be the expected ratio of atoms A to atoms B, in the alloy A_xB_{1-x}. µ-ATOMS is aimed at uncovering the physics determining SRO, knowledge of the existing role of SRO on semiconductor properties, and new techniques to manipulate and control SRO. This is a knowledge base that can enable a scaled-up, reliable, and cost-effective sequence of operations for manufacturing semiconductor structures and devices from the bottom-up.

The impact is a new science of deterministic positioning, with a codesign purpose to utilize the spatial arrangements of atoms utilize spatial arrangements of atoms to synthesize novel heterostructures and graded morphologies using a single material, purposely ordered to form *(Figure 1)*: ***(i)*** SRO of atoms that defines low loss quantum wells, wires, dots, and corresponding photonic functions; ***(ii)*** different configurations of SRO that can be switched from one to the other as memory elements that truly converges transistors and memory, enabling facile in-memory computing and drastically increased energy efficiency; ***(iii)*** GeSn as a topological quantum material with SRO that harnesses and controls topological states for low-loss electrical transport; ***(iv)*** SRO of defects, such as vacancies, to lower electron-phonon scattering; and ***(v)*** domains of SRO that impact thermal transport much more than electrical transport, creating new opportunities for heat to electricity conversion. It presents opportunity for new microelectronic technology, leveraging a fundamental understanding of the underlying physics of the ordering of atoms in crystals, for new science on a silicon platform.

This mission will be realized by a team of researchers who are currently leading the experimental and modeling research breakthroughs on Group IV GeSn and SiGeSn semiconductor materials and who seek the underlying physics and chemistry principles for the ordering of atoms in semiconductor alloys as the knowledge base for a new technique for the synthesis for semiconductor properties and structures. The approach is rooted in a "Center Structure of Four Integrated Thrusts" *(Figure 1)* which parallel our four EFRC goals. The integrated thrusts and research goals of the Center are:

1. **Model both material and structure** to guide fabrication, and measurement of SRO in Group IV semiconductors. We are building on our early modeling results to precisely arrange Group IV (Si, Ge, Sn, Pb) crystal structures to discover and predict **(i)** the type and degree of SRO, **(ii)** the dependence on growth parameters, and **(v)** the expected performance of functional structures, such as QWs, using SRO.
2. **Develop new synthesis tools and techniques** to control and prepare Group IV semiconductors with different types and degrees of SRO. We are utilizing two different fabrication methods, spontaneous and stimulated, to achieve growth of different degrees of SRO and control over the spatial arrangement of SRO domains. Both methods rely on our pioneering new spontaneous and stimulated growth techniques, such as, amorphous crystallization, and Atomically Precise Advanced Manufacturing.
3. **Explore new characterization tools** to determine the ability to measure the type and degree of SRO. For example, we are leveraging our results, such as, using atomic probe topography and new simultaneous scanning transmission electron microscopy and Raman capabilities, to reveal the degree and type of SRO. We are using these tools to determine the correlation between SRO and material electrical and optical properties which are compared with our modeling predictions.
4. **Control SRO in Group IV semiconductor alloys for transformative opportunities**. We are determining the ability to control the type and degree of SRO in Group IV SiGeSnPb crystals by applying what we learn in thrust 1-3 to co-design and synthesize novel functional structures (Figure 1). This includes synthesizing controlled spatial arrangements of SRO domains to co-design quantum wells, wires, dots, waveguides, lasers, and transistors with memory.

The outcome from the µ-ATOMS EFRC is to demonstrate fundamental understanding and precision manipulation of SRO in Group IV semiconductor alloys as a new tool and to deliver new science and novel device concepts on a silicon chip.

µ-ATOMS	
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