Electronic Materials: Physics and Applications

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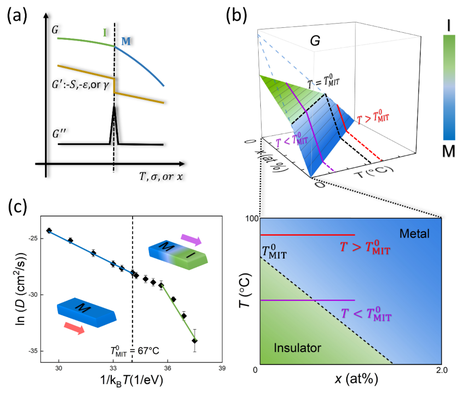
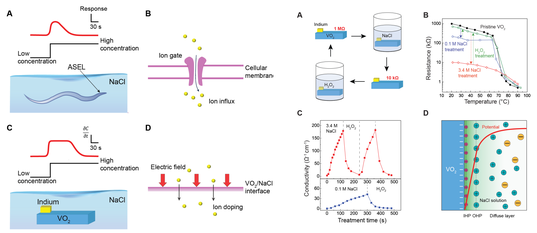
Introduction

The Wu Group explores **fundamental physics** and **new applications** of low-dimensional materials, layered transition metal dichalcogenides, phase change materials, and their interfaces. We aim to understand the influence of defects, doping, microstructuring and external stimuli on the electronic and thermal properties and performance of these materials, for potential applications in sensing, energy saving and harvesting, optics and electronics.

Phase Transition and Phase Change Materials



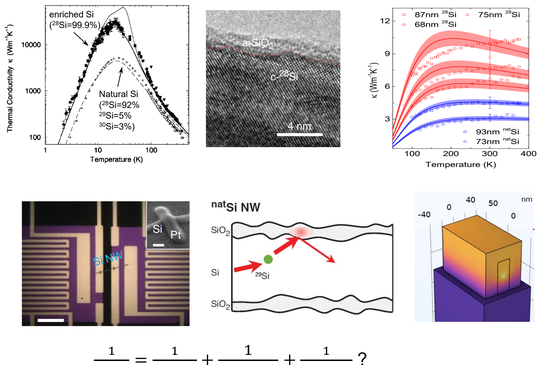
In first-order **phase transitions**, the second derivatives of Gibbs free energy (specific heat and compressibility) diverge at the transition point, resulting in an effect known as super-elasticity along the pressure axis, or super-thermicity along the temperature axis. Here we report a chemical analogy of these singularity effects along the atomic doping axis, where the second derivative of Gibbs free energy (chemical susceptibility) diverges at the transition point, leading to an anomalously high energy barrier for dopant diffusion in co-existing phases, an effect we coin as super-susceptibility. The effect is realized in hydrogen diffusion in vanadium dioxide (VO_2), where hydrogen faces three times higher energy barrier when it diffuses across a metal-insulator domain wall in VO_2. The super-susceptibility and resultant retarded atomic diffusion are expected to exist universally in all phase transformations where the transformation temperature is coupled to chemical composition, and inspires new ways to engineer dopant diffusion in phase-coexisting material systems. - *Cai, et al, publication pending (2024).*



Biomimetics: spontaneous ion exchange with aqueous electrolytes. We discovered that merely soaking a VO_2 film into an aqueous electrolyte (e.g., a NaCl solution) introduces its MIT. The effect is bias-free, rapid, non-volatile and reversible, offering simultaneous sensing and memorization functions, and explained by cation exchange at the solid/liquid interface driven by electric fields in the Helmholtz layer. The effect is also ion species selective (e.g., Na^+, K^+, Cs^+), promising as basic elements for wetware in brain-like computing and simulation of neuroplasticity. - *Guo et al, publication pending (2024)*

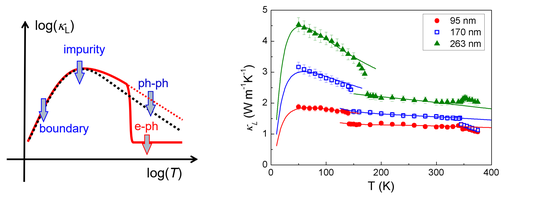
Phys. Rev. Lett., 129, 245701 (2022); Science, 355, 371 (2017); Phys. Rev. B Rapid Commun., 102, 041120(R) (2020); PNAS, 116, 07576 (2019); Nano Lett., 17, 2512 (2017); PNAS, 116, 9186 (2019); Nature Commun., 11, 5770 (2020).

Thermal and Thermoelectric Transport

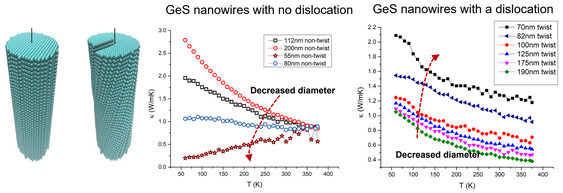


$$\frac{1}{\tau_{total}} = \frac{1}{\tau_{ph-ph}} + \frac{1}{\tau_{defects}} + \frac{1}{\tau_{surface}} ?$$

Giant Isotope Effect of Thermal Conductivity in Silicon Nanowires. Isotopically purified semiconductors potentially dissipate heat better than their natural, isotopically mixed counterparts as they have higher thermal conductivity (κ). But the benefit is low for Si at room temperature, amounting to only ~10% higher κ for bulk ^{28}Si than for bulk natural Si (^{nat}Si). We show that in stark contrast to this bulk behavior, ^{28}Si (99.92% enriched) nanowires have up to 150% higher κ than ^{nat}Si nanowires with similar diameters and surface morphology. Using a first-principles phonon dispersion model, this giant isotope effect is attributed to a mutual enhancement of isotope scattering and surface scattering of phonons in ^{nat}Si nanowires, correlated via transmission of phonons to the native amorphous SiO_2 shell. The work inspires potential applications of isotopically enriched semiconductors in microelectronics. - *Ci, et al, Phys. Rev. Lett., 128, 085901 (2022).*



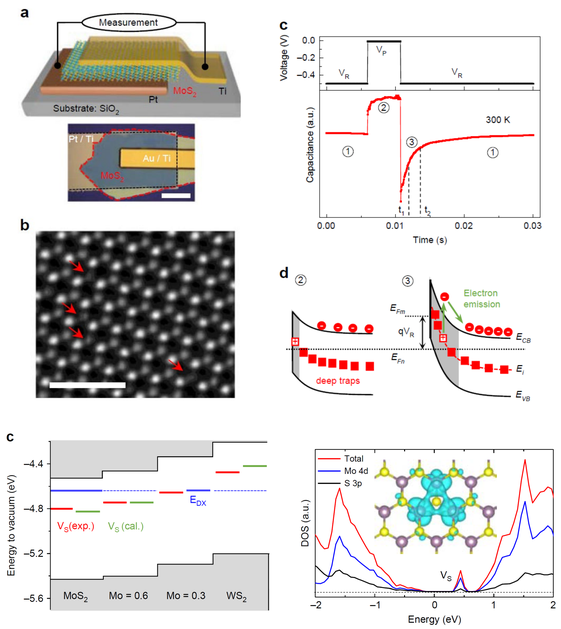
Anomalously Suppressed Thermal Conduction by Electron-Phonon Coupling in Charge-Density-Wave Tantalum Disulfide. Charge and thermal transport in a crystal is carried by free electrons and phonons (quantized lattice vibration), the two most fundamental quasiparticles. Above the Debye temperature of the crystal, phonon-mediated thermal conductivity (κ_L) is typically limited by mutual scattering of phonons, which results in κ_L decreasing with inverse temperature, whereas free electrons play a negligible role in κ_L. We discovered an unusual case in charge-density-wave tantalum disulfide (1T-TaS_2), in which κ_L is limited instead by phonon scattering with free electrons, resulting in a temperature-independent κ_L. In this system, the conventional phonon-phonon scattering is alleviated by its uniquely structured phonon dispersions, while unusually strong electron-phonon (e-ph) coupling arises from its Fermi surface strongly nested at wavevectors in which phonons exhibit Kohn anomalies. - *Liu, et al, Adv. Sci., 7, 1902071 (2020).*



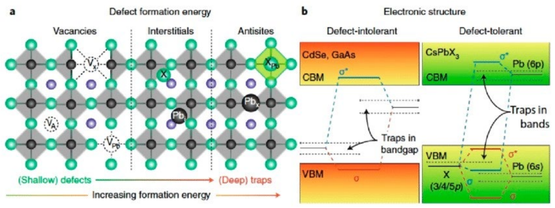
Abnormal thermal conduction in GeS nanowires with a single screw dislocation in the core. In twisted (dislocated) nanowires, thermal conductivity (*k*) shows unusual, opposite dependence on nanowire radius than that in normal nanowires. Dislocation core is found to host distinct atomic-scale structures and phonon properties. – *Liu et al, Publication in review (2024).*

Phys. Rev. Lett., 128, 085901 (2022); Science, 355, 371 (2017); Adv. Sci., 7, 1902071 (2020); Nature Commun., 13, 4901 (2022); Appl. Phys. Lett. , 121, 022201 (2022); J. Appl. Phys., 131, 025101 (2022); Nature Commun., 11, 6028 (2020).

Defects, Doping and Alloying



Chemical trends of deep levels in van der Waals Semiconductors. Properties of semiconductors are largely defined by crystal imperfections including native defects. Van der Waals (vdW) semiconductors, a newly emerged class of materials, are no exception: defects exist even in the purest materials and strongly affect their electrical, optical, magnetic, catalytic and sensing properties. However, unlike conventional semiconductors where energy levels of defects are well documented, they are experimentally unknown in even the best studied vdW semiconductors, impeding the understanding and utilization of these materials. We directly evaluated deep levels and their chemical trends in the bandgap of MoS_2, WS_2 and their alloys by transient spectroscopic study. One of the deep levels is found to follow the conduction band minimum of each host, attributed to the native sulfur vacancy. A switchable, DX center - like deep level has also been identified, whose energy lines up instead on a fixed level across different hosts, explaining a persistent photoconductivity above 400 K. - *Ci et al, Nature Commun., 11, 5373 (2020).*



Semiconductor defect states are derived from different atomic orbitals. Depending on their location in the band structure of the host, the host exhibits different degree of tolerance to these defects. We investigate the fundamental defect physics of various semiconductors including hybrid perovskites for better understanding of their properties in device applications.

Nature Commun. 11, 5373 (2020); Phys. Rev. Lett., 125, 226403 (2020); Nano Lett., 23, 1445 (2023); Nano Lett., 22, 9027 (2022); Phys. Rev. Lett., 126, 223601 (2021); Nature Electronics, 5, 505, (2022).

Acknowledgments

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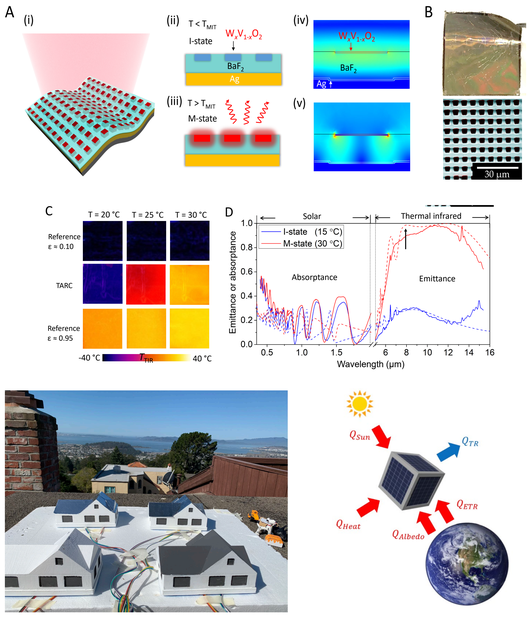
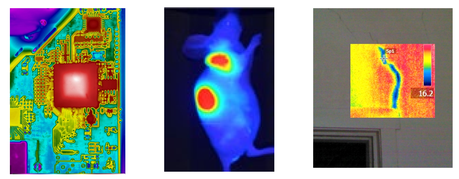
Sensing and Energy Applications

$P_{rad}(T) = \int_0^\infty B(T,\lambda)\cdot\varepsilon(\lambda)d\lambda = \varepsilon\,\sigma T^4$, where $B(T,\lambda) = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/(\lambda k_B T)}-1}, \sigma = \frac{2\pi^5 k_B^4}{15c^2h^3}$, and ε is emissivity of thermal radiation



Temperature-adaptive radiative coating for all-season household thermal regulation. The sky is a natural heat sink that has been extensively used for passive radiative cooling of households. A lot of focus has been on maximizing the radiative cooling power of roof coating in the hot daytime using static, cooling-optimized material properties. However, the resultant overcooling in cold night or winter times exacerbates the heating cost, especially in climates where heating dominates energy consumption. We approached thermal regulation from an all-season perspective by developing a mechanically flexible coating that adapts its thermal emittance to different ambient temperatures. The fabricated temperature-adaptive radiative coating (TARC) optimally absorbs the solar energy and automatically switches thermal emittance from 0.20 for ambient temperatures lower than 15°C to 0.90 for temperatures above 30°C, driven by a photonically amplified metal-insulator transition. Simulations show that this system outperforms existing roof coatings for energy saving in most climates, especially those with substantial seasonal variations. - *Tang et al, Science, 374, 1504(2021)*



TARC and similar structures can be also made to amplify ultralow thermal radiation contrasts, serving as a **thermal imaging sensitizer coating**, which may find applications in high-sensitivity detection of hot/defect spots in circuit boards for trouble shooting, thermographic diagnostics of tumor or unusual biological activities under skin, and IR inspection of hidden defects in buildings/bridges. – *Tang et al, Sci. Adv., 6, eabd8688 (2020)*

Science 374, 1504-1509 (2021); Cell Reports Physical Science, 3, 101066 (2022); Materials Today, 45, 120 (2021); Science Advances, 6, eabd8688 (2020); Adv. Mater., 1907071 (2020).