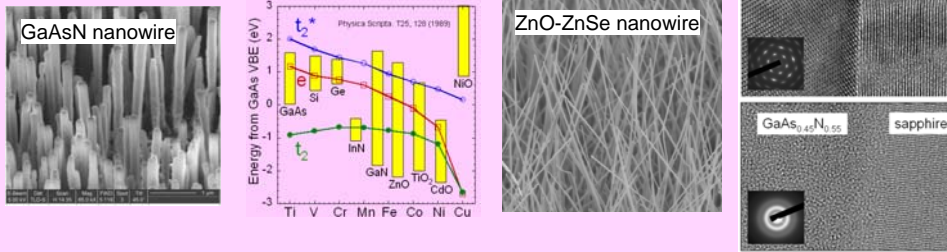


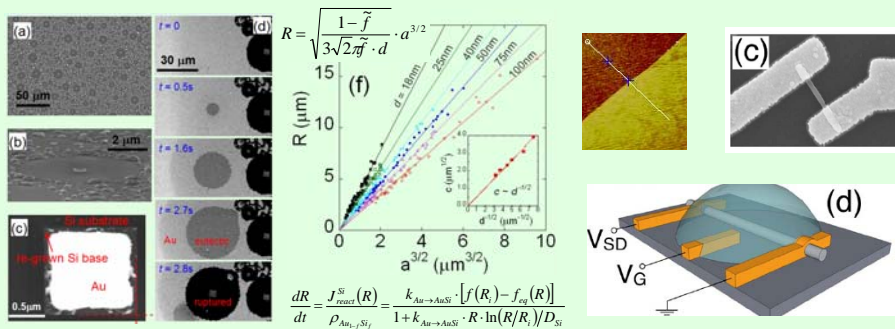
Objectives: Develop new multi-functional materials and material systems with electronic structure tunability and / or dynamical responsivities for innovative energy and device applications; understand the physical mechanisms governing the properties through theoretical analysis and numerical simulation.

highly mismatched semiconductors



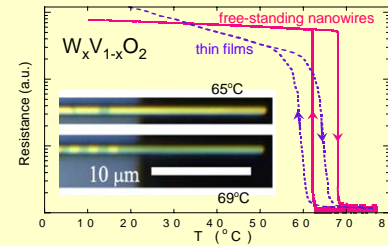
sp electrons: electronic band structure tunabilities.
d-electrons or highly mismatched impurities: strong localization and correlation.
Non-equilibrium semiconductor alloys for thermoelectric and photovoltaic applications.

low-dimensional alloys and interfaces

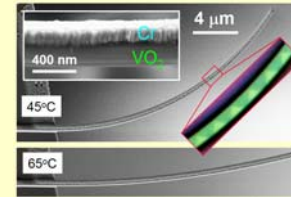


Ultra-fast, surface-enhanced atomic self-diffusion in ultra-thin AuSi eutectic liquids.
Graphene: point defects and electromechanics.
Solar and electrochemical activity at single semiconductor-electrolyte interface.

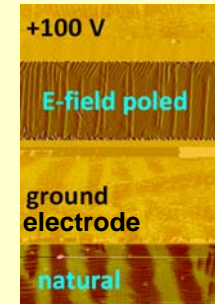
nanomaterials with multi-functional phase transitions



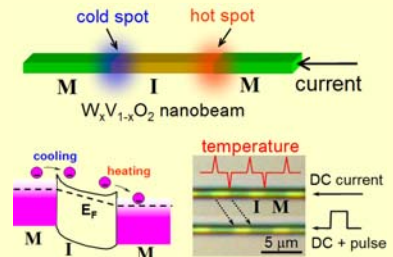
Single-domain metal-insulator transition in single-crystal $W_xV_{1-x}O_2$ nanowires allowing probe of intrinsic phase transition physics and domain dynamics.



Structural functionality: much higher responsivity to external stimuli, promising application in sensing, transduction, actuation and energy harvesting.

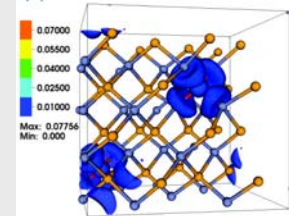
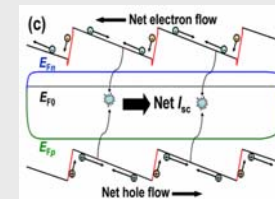
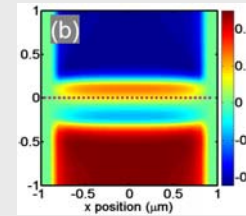


Multiferroics: controlling magnetism with electric field in mechanically confined mixed-phase $BiFeO_3$ structures.



Electrothermal functionality: localized Peltier heating and cooling at nm-thick M-I domain walls as mobile, rewritable Schottky junction for nanoscale thermal management in microfluidics and biology.

numerical simulation and fundamental understanding



$$\mathbf{j}_n(\mathbf{r}) = -\sigma_n(\mathbf{r})\nabla V(\mathbf{r}) - eD_n\nabla n(\mathbf{r}) - \sigma_n(\mathbf{r})S_n(\mathbf{r})\nabla T(\mathbf{r})$$

Modeling electrodynamics and electromechanics to understand nanoscale physical behavior of materials and devices.