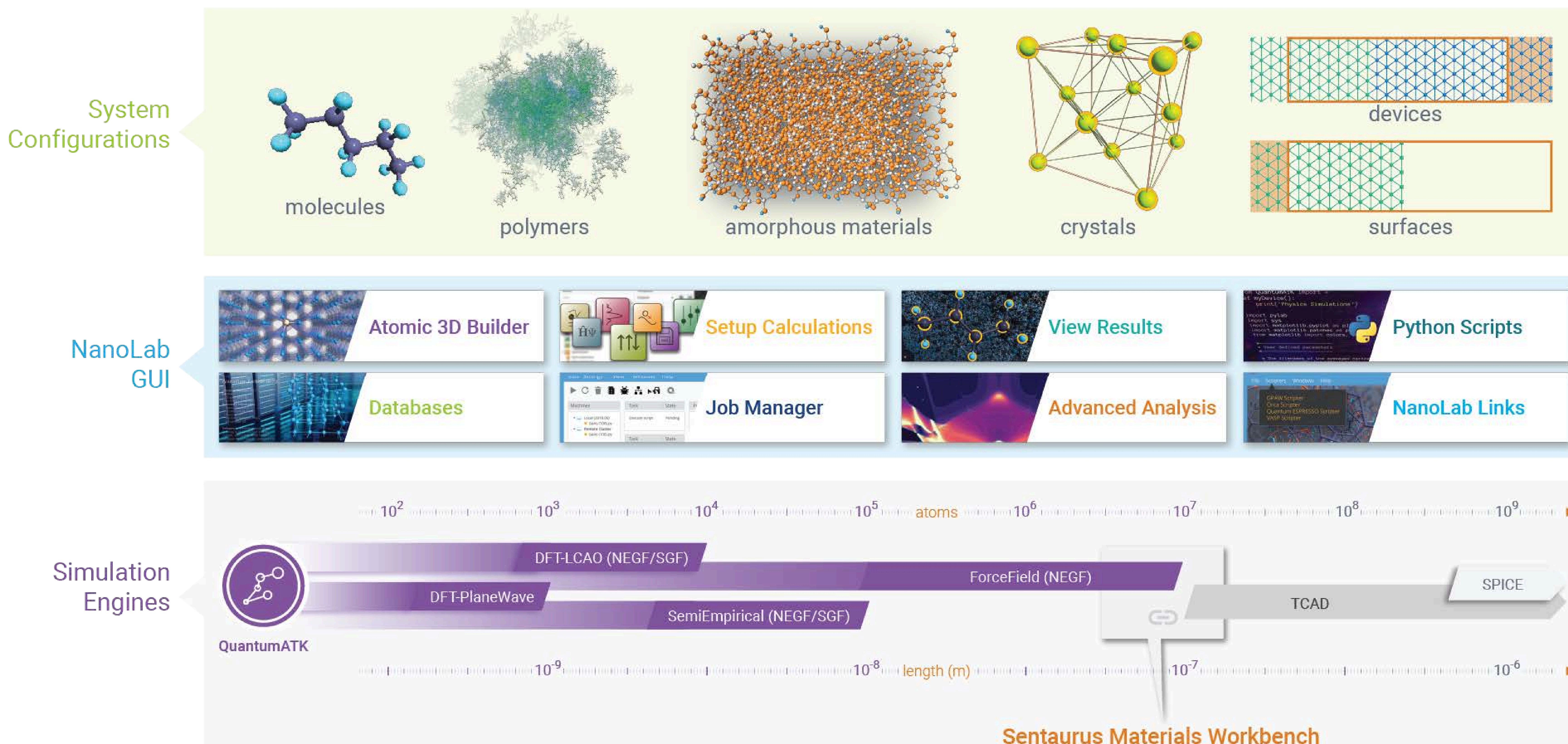




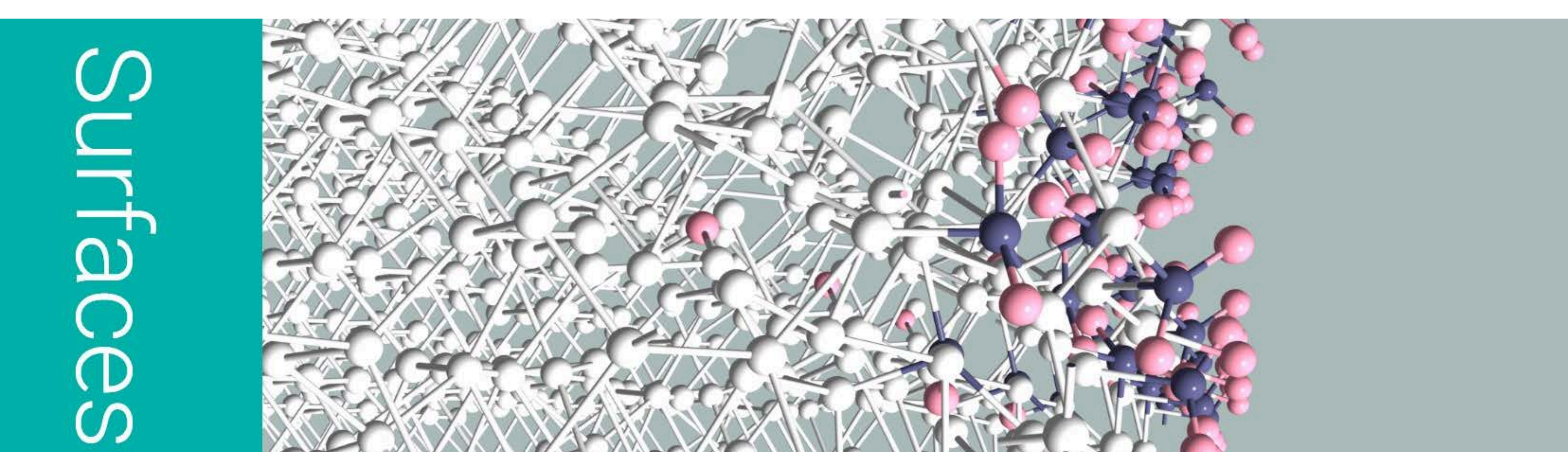
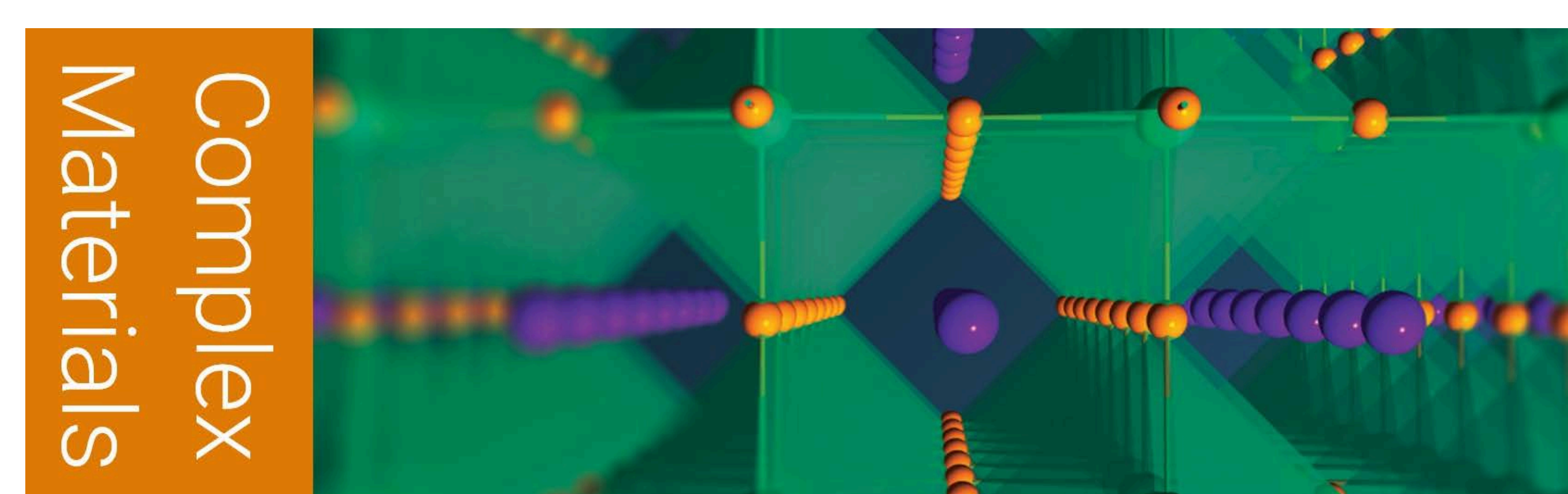
# Synopsys QuantumATK for Atomistic Modelling and Simulation of Nano-Materials/Devices



## Material Properties

### Bulk Materials, 2D/1D Nanostructures, and Surface

- Electronic (band structure, effective masses, work functions, mobility, etc.)
- Defect formation energies, diffusion constants, etc.
- Thermal (phonon band structures)
- Thermoelectric, Optical, Magnetic, Mechanical, Piezoelectric
- Surface chemistry in electrostatic fields and surface states

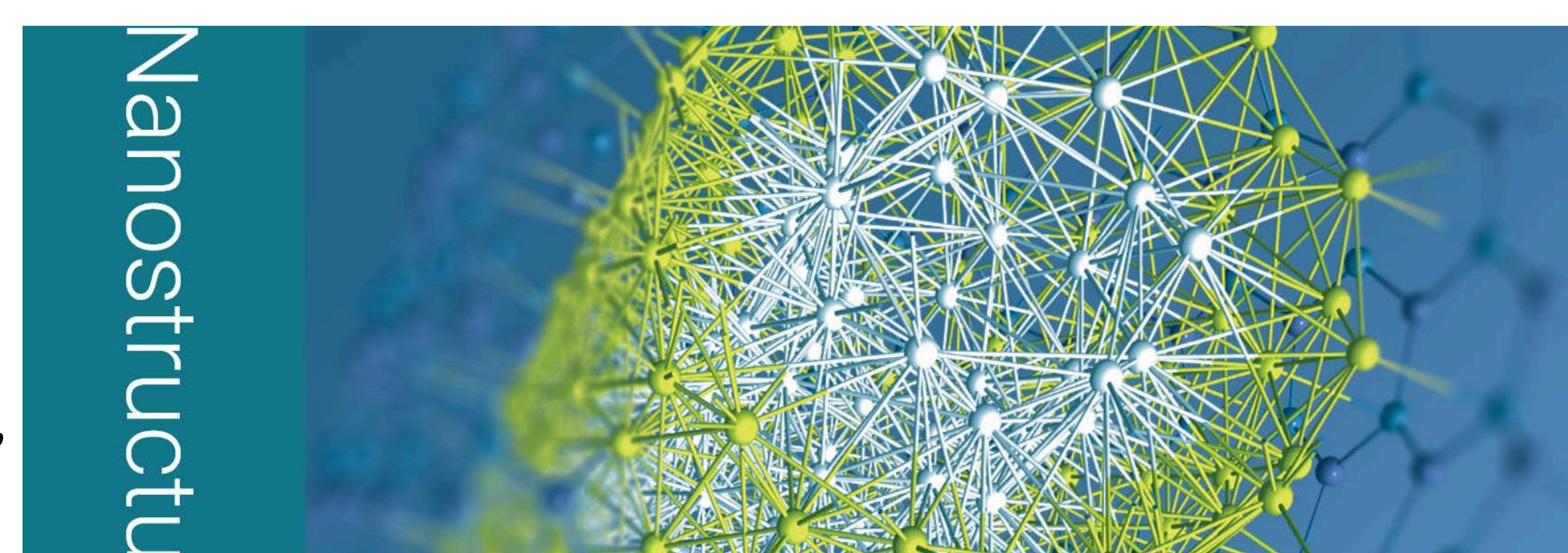


### Interfaces between Materials

- M|M, M|I, S, etc. (M: Metal, S: Semiconductor, I: Insulator)
- Grain boundaries
- Band alignment and offset at interfaces
- Contact (thermal) resistance
- Schottky barriers
- Interfaces in solar cells

## Emerging Nano Devices

- Electronic and thermal transport analysis
- Current-voltage characteristics (I-V curve)
- Transistor characteristics
- Leakage Current
- Electron-phonon scattering effects
- Architectures: FinFETs, TFETs, vertical/horizontal nanowires, nanosheets, nanotubes, etc.

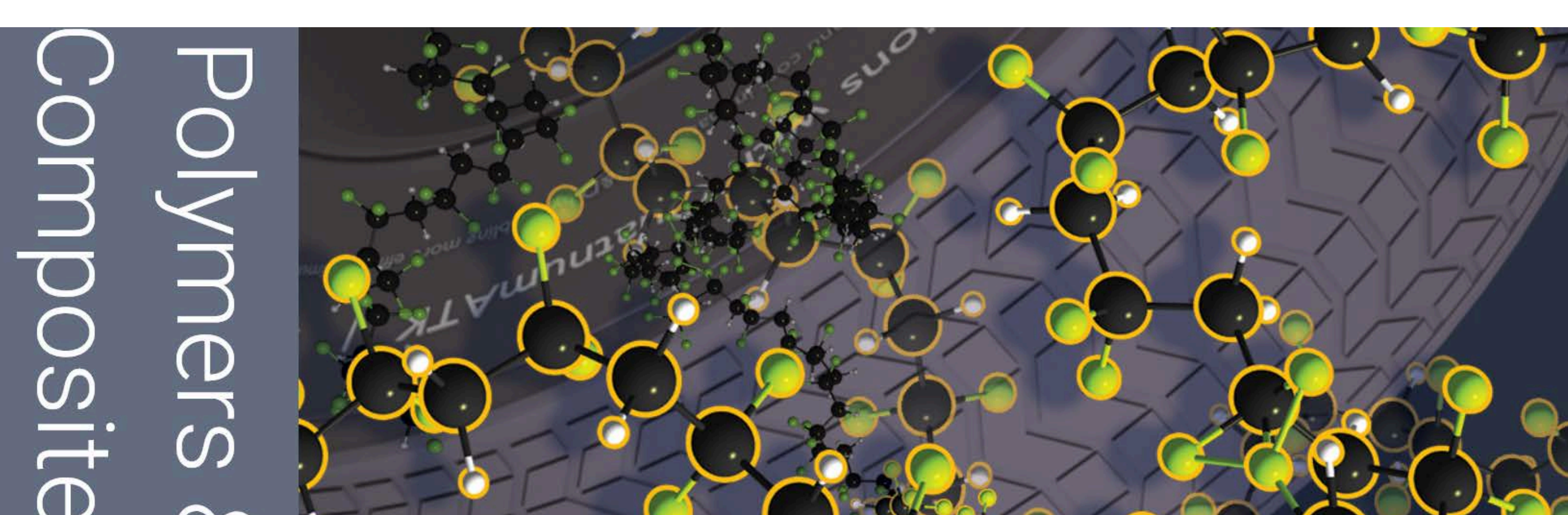
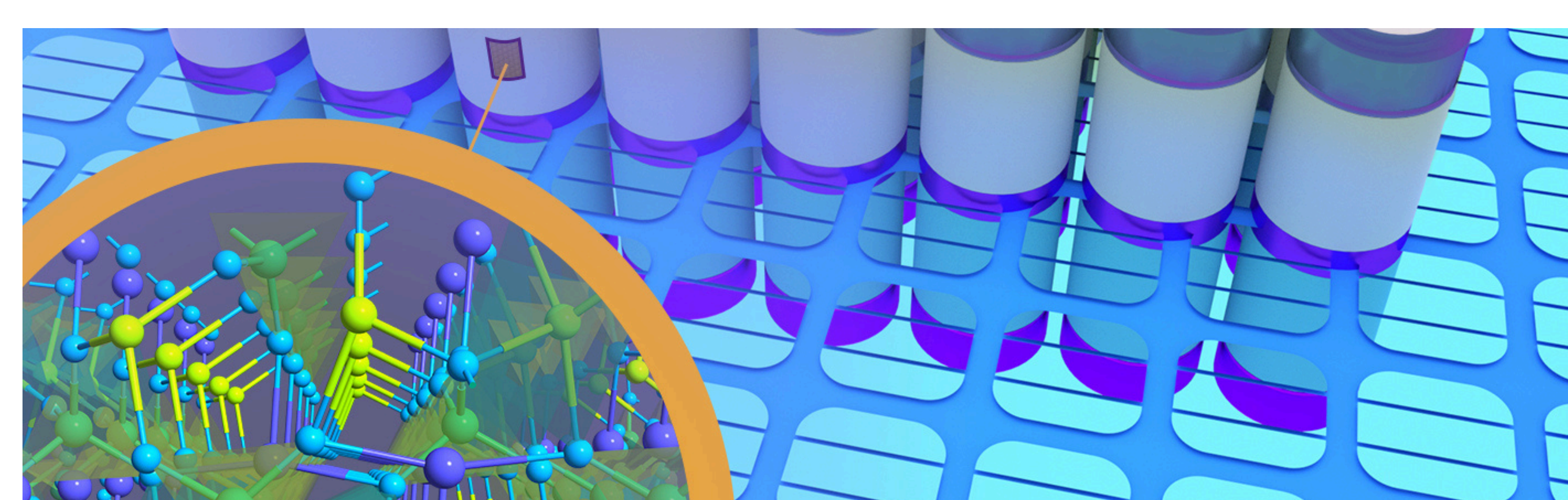


## Spintronic Devices

- Tunnel magnetoresistance and Parameter Sweeps and Optimization
- Interfacial resistance at the junction
- MRAM and Spin transfer torque (STT)-MRAM
- Topological insulators
- Spin-Polarized Calculations
- Transport Calculations
- Visualization and Analysis

## Batteries and Energy Storage Devices

- Li-ion, Li-air, Li-S, and other battery types
- Li-ion diffusion rates
- Open-circuit voltage profile during the cell discharge
- Interfaces with/without vacancies and their effects on electronic transport in batteries
- Charge and Energy Storage Mechanisms



## Polymers and Composite

- Linear homo-polymers, co-polymers and polymer blends
- Polymer/Molecule blends. Example: Photo acid generator (PAG) molecules in PMMA matrix.
- Polymer/Polymer and Polymer/Inorganic interfaces.
- Polymer/Nanoparticle composites. Example: Polymer melts with SiO<sub>2</sub> nanoparticles.
- Parameter Setup and Polymer Equilibration and Simulation Methods

