Multiscale Modeling of Electronic Materials (MSME) Collaborative Research Alliance (CRA)

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MSME CRA TOP-LEVEL GOALS

Develop capability to characterize, compute and predict multi-scale phenomena in electronic materials concurrently in space & time at fidelity required to develop electronic materials for the Army

- Drive forward and expand the fundamental understanding in the area of multi-scale/multidisciplinary materials behavior to directly improve the performance of electronic materials
- Execute a focused basic research program to design electronic materials for Army needs
- Create a framework that enhances and fosters cross disciplinary and cross organizational collaboration that brings a team of academia, industry and government together to address critical focused research in Multiscale Modeling of Electronic Materials

Focus on three electronic materials research areas:

- Electro chemistry
- Hybrid photonics
- Heterogeneous electronics

Develop validated multiscale models for:

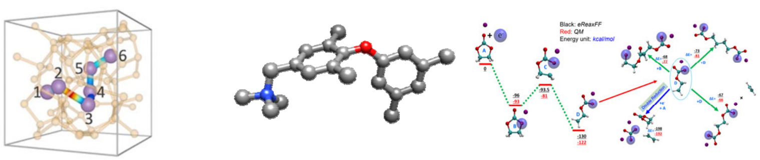
- Transport, interfaces & defects within semiconductor & energy conversion devices
- Growth, processing, and synthesis of heterogeneous materials
- Use uncertainty-quantified models and large scale parallel computing to predict reliable material and eventually device properties.

ELECTROCHEMICAL DEVICES

Mission Objectives: Design of materials that will enable energy storage devices with improved energy and power densities, cycle and storage life, safety and cost.

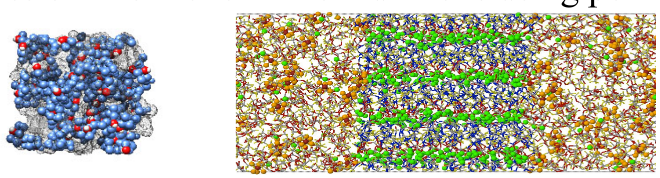
Approach: Multiscale modeling tools that couple key length and time scales and include:

→*Ab initio* calculations and reactive MD simulations (eReaxFF)



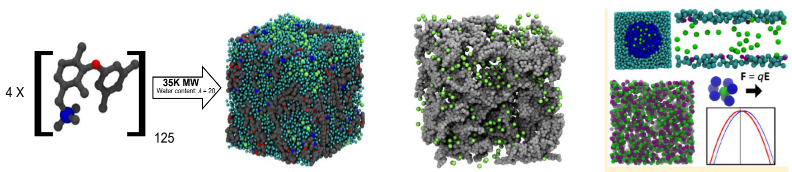
1-2 nm,
ps - ns

→Classical atomistic MD simulations using polarizable force fields



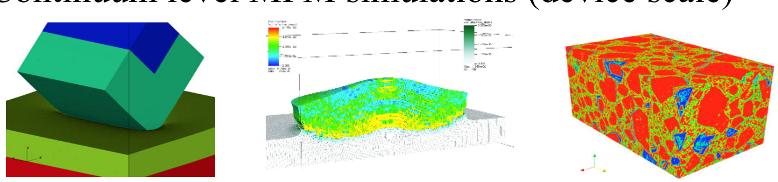
2-10 nm,
10 -100 ns

→Coarse-grained molecular simulations



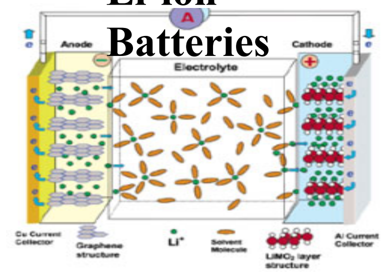
10 -100 nm,
100ns - μs

→Continuum level MPM simulations (device scale)

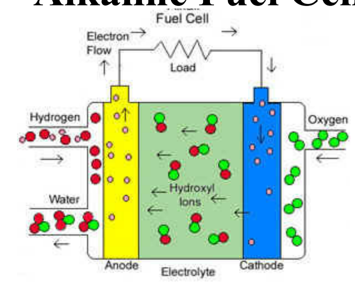


100nm - mm,
μs - s

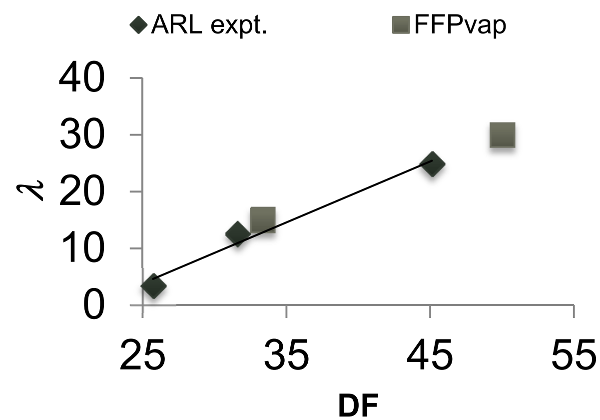
Li-ion Batteries



Alkaline Fuel Cell



Experimental validation by ARL efforts



Understanding how mechanics and electrochemistry couple at multiple scales to influence the properties of new materials

CROSS-CUTTING THEMES

Mission Objectives: **Design of cross-cutting multi-scale uncertainty-aware tools that will enable design of materials with quantifiable understanding of both performance and robustness.**

Approach: **Development of robust multiscale modeling tools that are coupling all key length and time scales, chemistry and physics and include:**

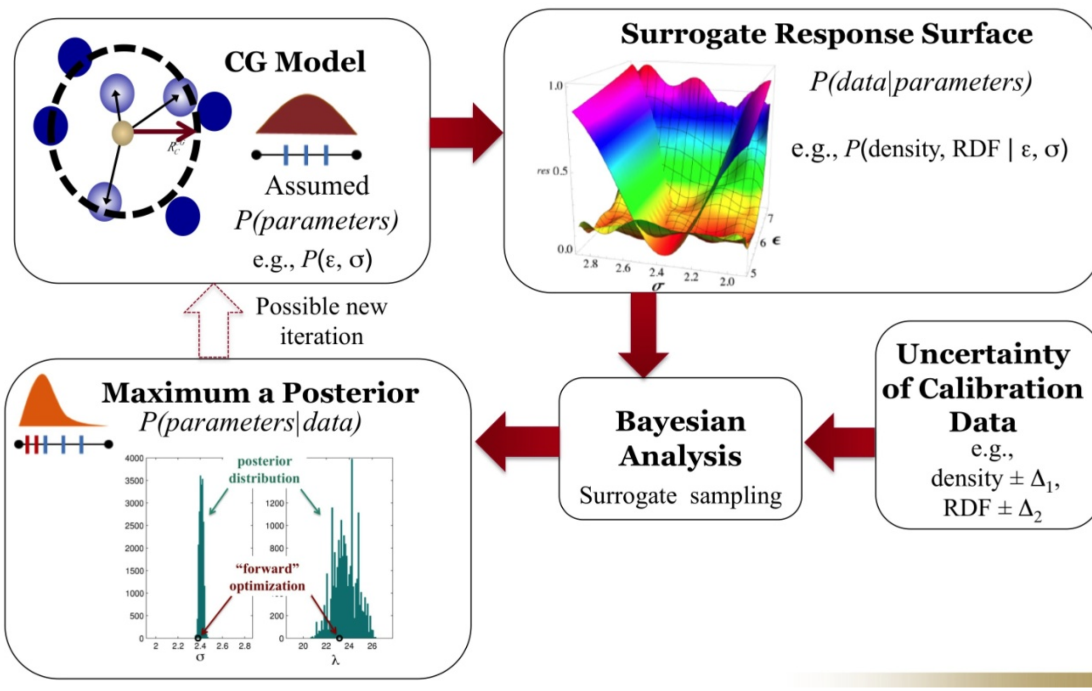
-High level (accurate) *ab initio (DFT)* calculations

- Uncertainty propagation for heterogeneous material

-Development of Rigorous Uncertainty Quantification (UQ) for MD

-UQ-Driven Coarse-grained MD simulations

-Continuum material point method (MPM) / MD multiscale multiphysics simulations



Quantifying Uncertainties Across the Scales For Robust Materials Design

HYBRID PHOTONICS

Mission Objectives: **Design of electronics and photonics materials that will enable the next generation of ARMY's electro-optics, communication, and energy management systems.**

Approach: **Development of a multi-physics hierarchy of modeling tools that encompass length and time scales from atoms to macroscopic systems.**

Atomistic Length/Time Scale

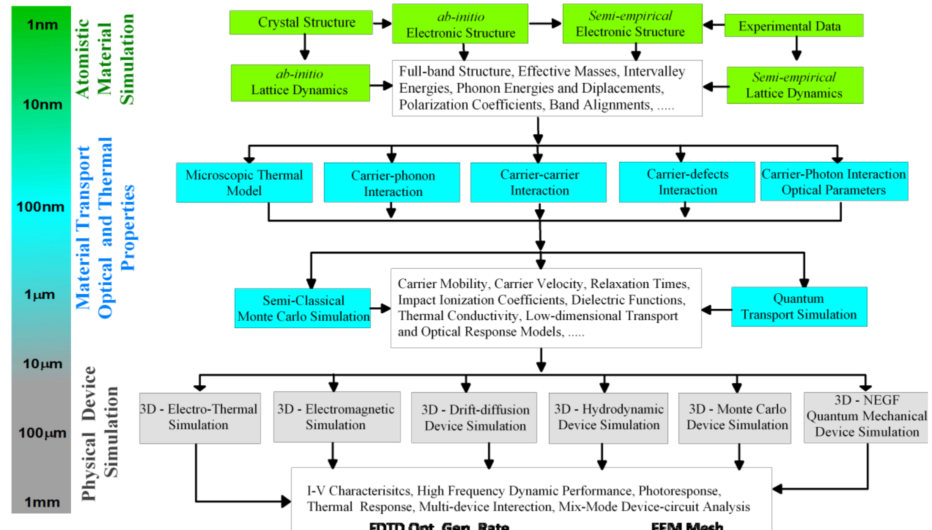
- *ab initio* structural and excited state calculations (DFT/HSE/GW).
- Computationally efficient semi-empirical atomistic models (SEPM/TB/KdP).

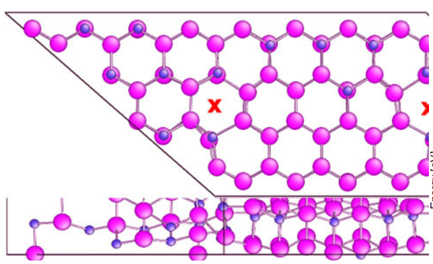
Mescoscopic Length/Time Scale

- Quantum mechanical transport models (QM-BTE).
- Quantum mechanical derived material properties (EGF).

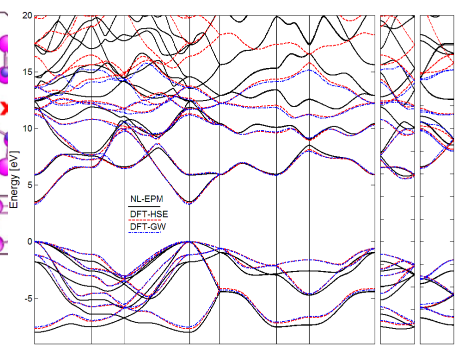
Macroscopic Length/Time Scale

- Hydrodyamic and drift diffusion transport model models.
- Surface and volume element electromagnetics.



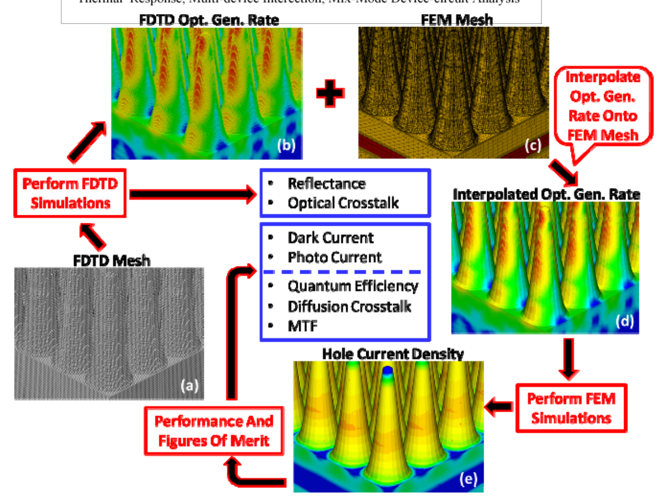


Extended Defects in and excited states calculation in GaN



GaN electronic structure UQ.

Coupled electronics and electromagnetic simulation of macroscopic systems with QM derived material properties.



HETEROGENEOUS ELECTRONICS

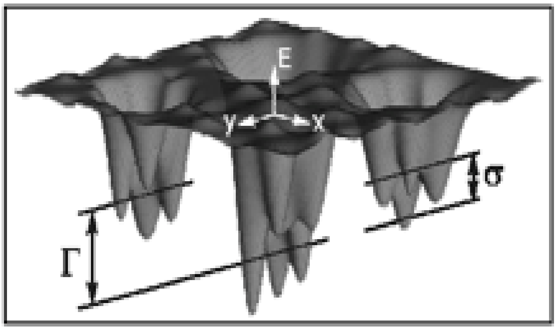
Mission Objectives: **Heterogeneous Electronic and Photonic Materials Design to enable energy efficient, robust and reliable electronics with enhanced speed, power handling, and ability to operate in extreme environments**

Approach: **Development of materials merit factors specific to device applications, developing multiscale modeling tools and multiscale characterization and validation technique to include:**

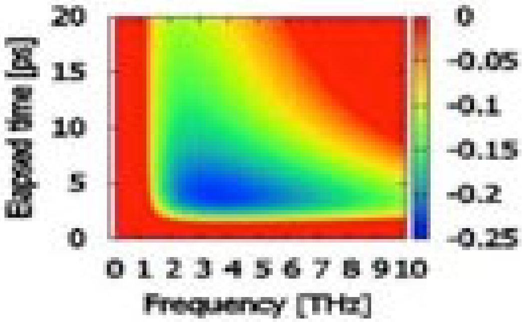
- advanced Monte Carlo techniques,

- 2D and 3D hydrodynamic simulations,

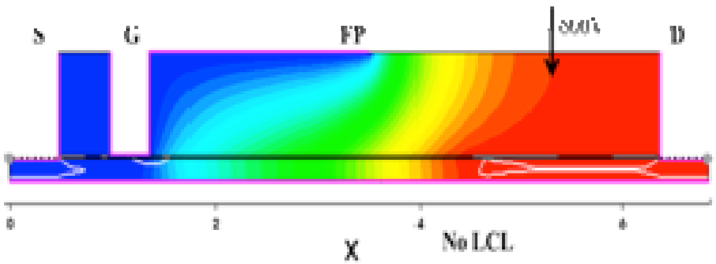
- nonlinear TLM simulations



Band edge in AlGaN
high efficiency UV LEDs



Gain and loss in far infrared
2D lasers



2D and 3D simulation of
high voltage switching
for energy efficient electronics