Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA)
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Class: 2020 – 2024

Mission Statement*: To achieve extreme electrical properties and phenomena through fundamental understanding of ultra wide bandgap materials – including synthesis and impurity incorporation, electronic structure at interfaces, electron - phonon interactions at high fields, and phonon mediated thermal transport, which will enable a resilient, smart electricity grid.*

A resilient, smart electricity grid is necessary to integrate multiple energy sources, power storage capabilities, and diverse electrical needs, and Ultra wide bandgap (UWBG) semiconductors have been identified as a crucial enabling materials technology. The UWBG semiconductor and dielectric materials (or 'Ultra' materials) present a new realm for high field transport, electron-phonon interactions, and heat transport. Understanding their novel properties will enable "reinventing the electricity grid" by providing efficient energy conversion and control (Smart Grid) and a significant reduction in size where a substation could be replaced by a suitcase-sized power converter (Resilient Grid).

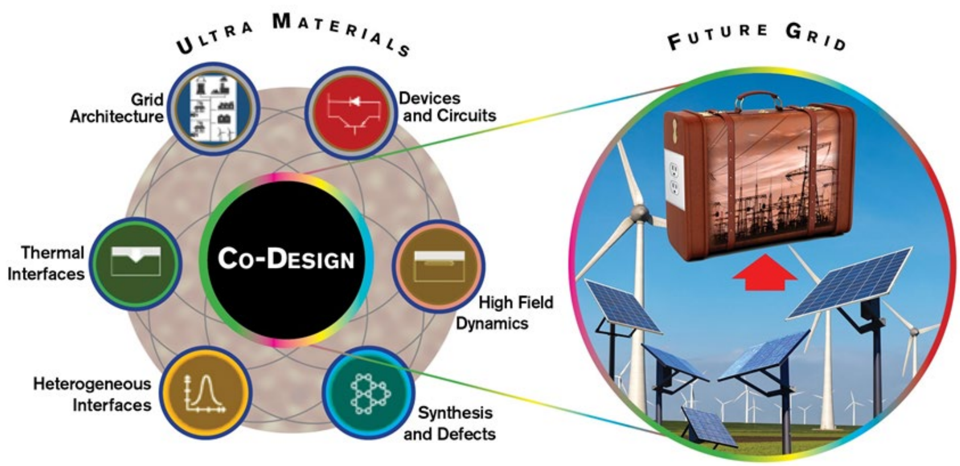

Figure 1. A Future Grid Co-Design Ecosystem will be established to enable communication across all levels of the science and technology.

The Mission of the Ultra EFRC is to understand fundamental phenomena in UWBG materials – including synthesis, defect and impurity incorporation, electronic structure at interfaces, interaction of electrons and atomic vibrations at high fields, to achieve extreme electrical properties, and efficient thermal transport. The Center will establish a co-design ecosystem enabling communication across all levels of the science and technology. The Center will focus on basic science challenges in four Thrusts: 1) growth, defects, and impurities, 2) heterogeneous interfaces, 3) carrier dynamics and high field transport, and 4) thermal energy transport and interfaces. The Ultra semiconductor materials of interest include cubic crystalline diamond, hexagonal crystalline AlN and the $B_xAl_{1-x}N$ alloy system which bridges the cubic and hexagonal crystal structure. The Ultra dielectric materials include oxide and fluoride thin films. The team brings together experts in non-equilibrium growth techniques, advanced microscopy, defect analysis, interface electronic states characterization, high field current transport, thermal properties, and thermal imaging measurements; this expertise is integrated with theory and modeling through a computational team that use *ab initio* first principles modeling, non-linear dynamics, self-consistent Monte Carlo heat transport, and high throughput simulations and materials informatics.

The research into new doping and interface configurations will be guided by high performance computing. As an example (Fig. 2), a multi-tiered computational screening approach will be used to identify low-energy, shallow-donor and acceptor defect configurations. The steps include importing the crystal structure, structural relaxation, high resolution simulation, high throughput simulations with correction terms included, computing formation energies, and selecting low formation energy shallow dopant configurations. Selected experimental results will be iterated into the process.

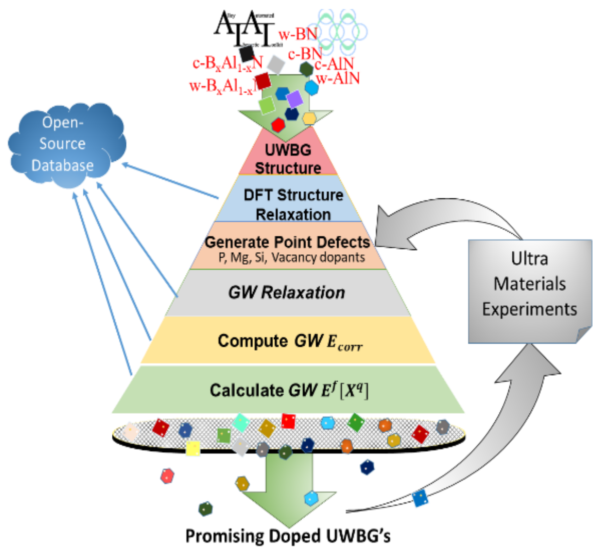

Figure 2. A high-throughput computational approach for identification of low formation energy and shallow donor and acceptor dopants in UWBG's.

The Ultra EFRC will establish a Future Grid Co-Design Ecosystem, and develop a knowledge-base of UWBG materials and properties to "Reinvent the Electricity Grid." The outcomes will include: 1) synthesis of cubic and hexagonal UWBG semiconductors, 2) experimental and theoretical understanding of defects and doping that transcends the different materials systems, 3) characterized UWBG heterostructures enabling new routes to doping that exploit the properties of interfaces, 4) development of a deep understanding of electric breakdown phenomena and high current transport in UWBG semiconductors, and 5) characterized interactions between electrons and atomic vibrations and understood the heat transport in UWBG materials and importantly, their interfaces. The research will provide a roadmap projecting how to achieve high breakdown field in the off-state, high current densities in the on-state, and highly efficient thermal conduction to minimize heating. The Future Grid Co-Design Ecosystem, will provide design simulation tools for a new generation of high power devices and power conversion modules and work with grid architect researchers to incorporate UWBG semiconductors in a Resilient, Smart Electricity Grid.

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