# Unravelling the Long-Life, High Capacity, and Ultrafast Charging Mechanisms Behind Mixed Niobium Oxide (XNO™) Battery Anode Materials

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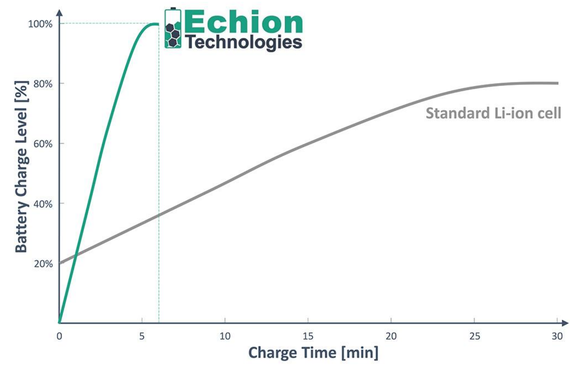
## Echion Technologies : Mixed Niobium Oxide (XNO™) Battery Anode Materials

Echion's XNO™ anode materials enable safe, long-life, fast-charging Li-ion cells

- ✓ 0 to 100% charge in 6 minutes or less
- ✓ Twice the energy density of LTO-based cells
- ✓ Safe operating voltage
- ✓ >10,000 cycle life
- ✓ Lowest total cost of ownership




Echion materials are available at scale for high performance Li-ion cells.

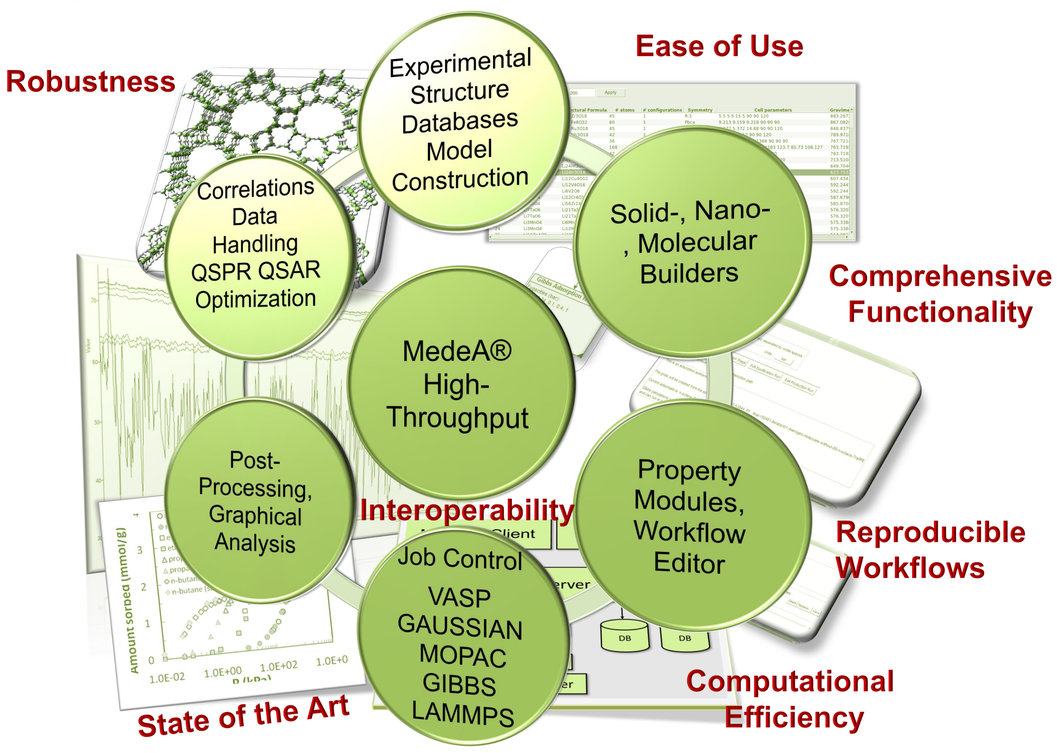
Contact Echion Technologies: info@echiontech.com

**Atomistic simulations with the *MedeA* software suite complements Echion's experimental work at low cost:**

- Search for the optimal mixing of niobium oxides with other lightweight elements to further improve XNO™
- Unveil the fundamental principles that enable the unprecedented reversible energy density and charging time of XNO™

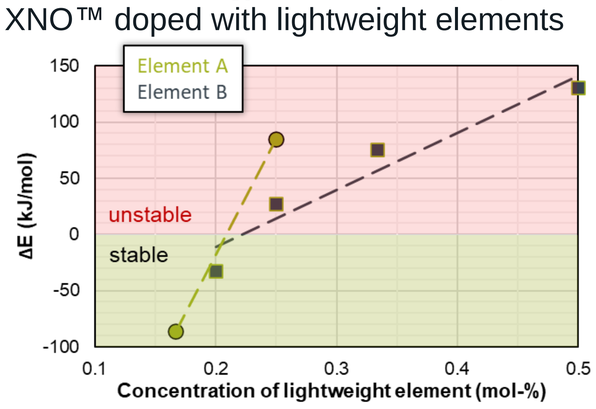
## *MedeA*® Software of *Materials Design*®: Atomic-Scale Simulations for Battery R&D

Calculate property data and obtain atomic-scale understanding for the design of battery materials



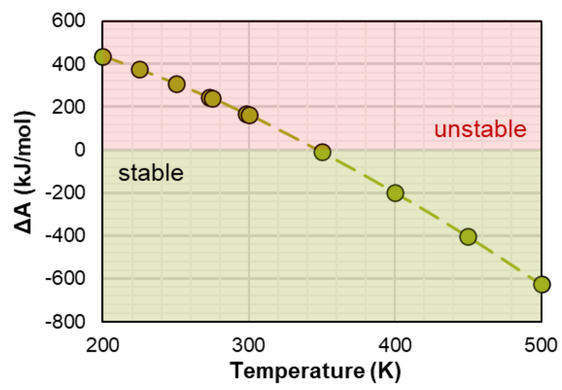

## Computational Thermodynamics of XNO™

Calculated energy of formation (ΔE) of XNO™ doped with lightweight elements




Compounds are stable at doping concentrations below 0.2 mol-%

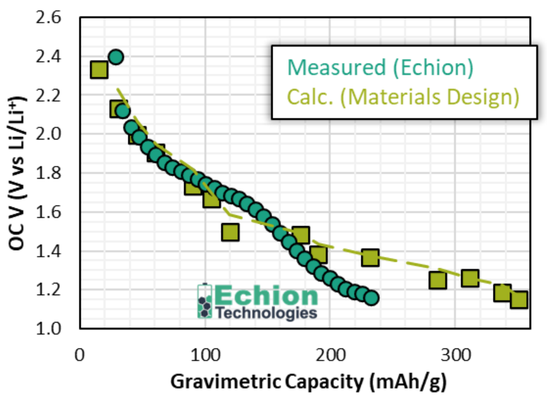
Calculated free energy of formation (ΔA) of XNO™ doped with 0.2 mol-% of a lightweight element




Doped XNO™ should be synthesized at temperatures larger than 400 K

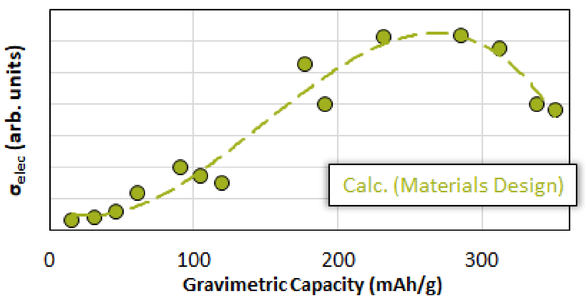
## Electrochemistry of Lithiated XNO™

Voltage profiles: Open circuit voltage (OCV) upon charging (lithiation)




Agreement between calc. and measured voltage profiles

Calculated trend of the electrical conductivity ($\sigma_{elec}$) upon lithiation



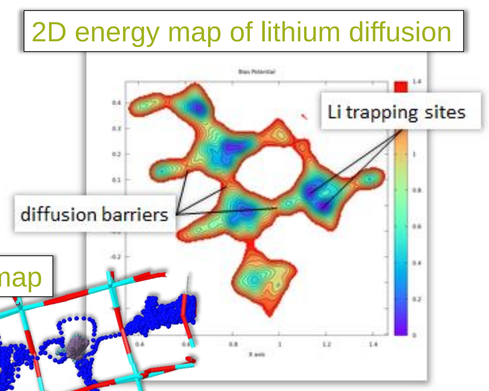

- XNO™ shows increasing metallic $\sigma_{elec}$ upon initial lithiation
- Lithiation beyond 280 mAh/g decreases $\sigma_{elec}$

## Simulation of Lithium Transport in XNO™

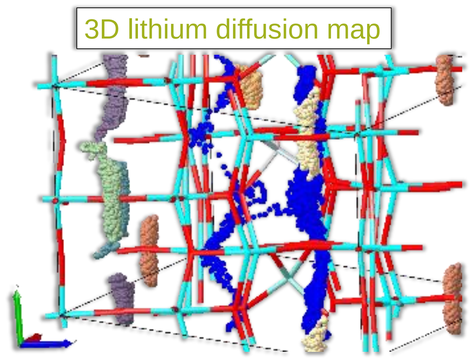
Calculated diffusion pathways reveal

- Fast lithium diffusion routes for rapid cycling
- Activation barriers to determine temperature dependent lithium diffusivity
- Lithium trapping sites to assess Coulomb efficiency

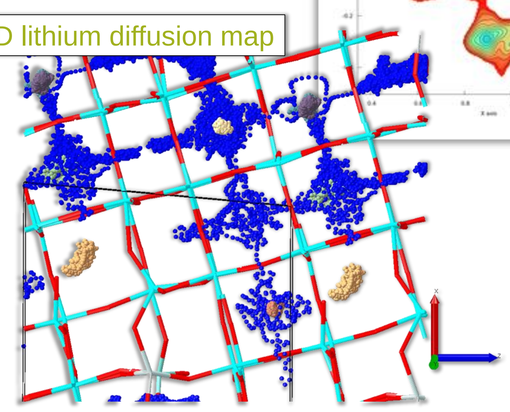
2D energy map of lithium diffusion




3D lithium diffusion map



2D lithium diffusion map



## *MedeA*® Calculates Properties for Electrodes, Electrolytes, Coatings, etc. & Interfaces Thereof

### Materials Fabrication

- Phase diagrams: miscibility vs separation
- Elasticity: ductility, brittleness, hardness
- Permittivity Dielectric constants
- Piezoelectricity
- Ion conductivity
- Thermal conductivity
- Thermal expansion
- Heat capacity

### Cycling behavior, fast charging

- Electrochemical stability vs degradation
- Phase transformation
- Volume change of particles
- Metal plating & stripping
- Interfacial stabilities/delamination
- Potential profiles
- Interphase morphology
- Interfacial contact
- Current density
- Electrical conductivity

### Diagnostics & Analysis

- IR & Raman Spectra
- UV-Vis Spectra
- XPS (core level shifts)
- Powder Diffraction Pattern

The Gateway to Computational Materials Science

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