CREI capabilities in Computational Materials Science

Unique expertise of faculty members (first-principles modeling)

- Alexei Buchachenko – spectroscopy of molecules at ultimate accuracy
- Sergei Tretiak – optoelectronic phenomena at nanoscale
- Andriy Zhugayevych – multiscale modeling of charge and energy flow

State of the art capabilities (energy and optoelectronic applications)

- DFT modeling of molecular and solid state, organic and inorganic materials
- Multiscale modeling of organic materials (inorganic is upcoming)
- Multilevel materials screening, computational design of materials
- Computational Materials Database, high-throughput calculations
- In collaboration with other CREIs: device modeling, machine learning approaches

Personnel, infrastructure, training

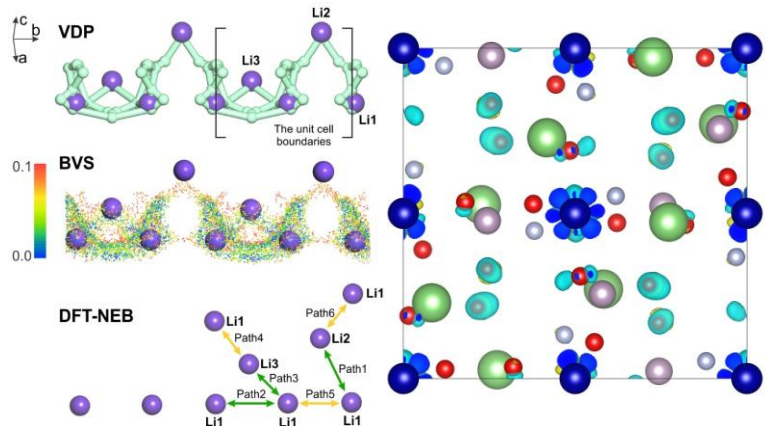
- 3 researchers, 2 PhD students, 2 MSc students, several part-time researchers
- VASP, Gaussian, LAMMPS, MOPAC + our own software incl. 2 published packages
- 200-core backup cluster + 100 cores/user + 2 terminals for students + databases
- Professional training for students and postdocs within the annual course “Computational Chemistry and Materials Modeling”

Selected recent research highlights

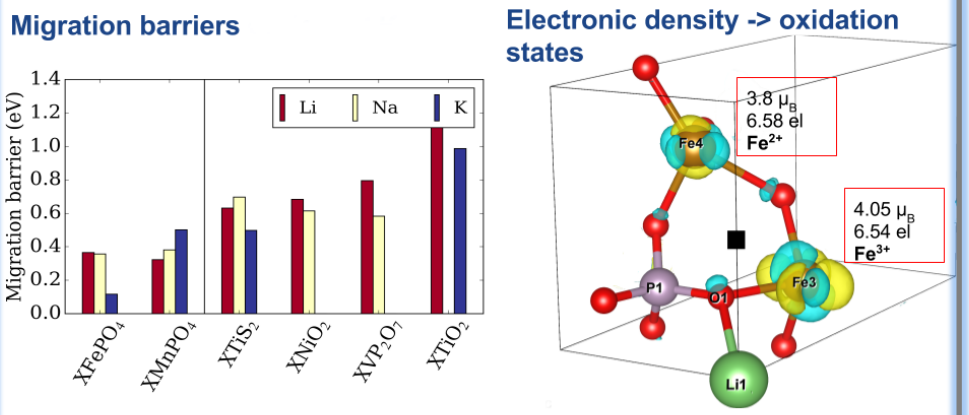
Inorganic cathodes for metal-ion batteries

(Zhugayevych, Aksenov, Fedotov)

Why only half of Li can be extracted from Li_2CoPO_4F (*J Phys Chem 2017*)



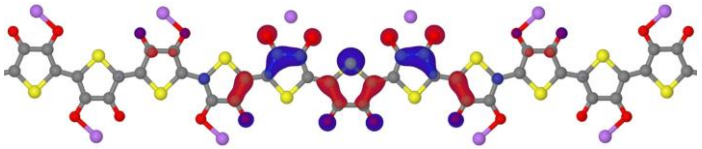
Computational design of Na- and K-ion cathodes



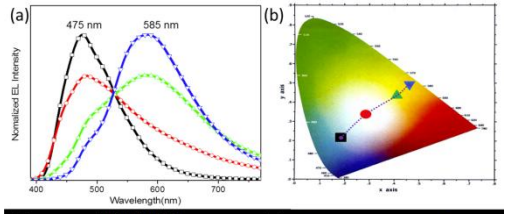
- redox potentials, volume changes, formation energies of antisites

Organic materials for energy and optoelectronics (funded externally)

(Tretiak, Zhugayevych, Kharlanov, Mazaleva, Naumov)



- Solar cells, *Annu Rev Phys Chem 66, 305 (2015)*
- Light emitters, *Chem Phys 481, 133 (2016)*
- Field effect transistors, *Chem Sci 8, 1146 (2017)*
- Photodetectors, *submitted to Adv Func Mater*
- Cathodes for batteries, *ground breaking work*
- Emerging biomaterials, *Adv Mater 27, 1908 (2015)*



Computational Materials Science Benchmarking

(prediction of device/material performance)

Application	Class of Materials / Reference	Scale (approach)	Property	Figures of Merit (best/CEE)			
				Automation	Diff.accuracy	Exp.uncertainty	Predictability
Batteries	Crystalline cathodes based on transition metal ionic compounds npj Comput Mater 2, 16002 (2016)	Single crystal (DFT)	Crystal structure	yes	no concerns	negligible	limited
			Average potential (~Voc)	yes	0.1 eV	0.1 eV	yes
			Voltage profile (~charge/discharge)	limited / no			limited
			Diffusion barriers (~power)	limited / no	0.1 eV	large	uncertain
		Single phase (classical MD)	*methods are under development*	no	uncontrolled		no
	Organic cathodes	Single phase (multiscale)	*ground breaking work, some calculations by IPCP partners*				
		Device	*not in CEE focus (ES?), some modeling by MSU partners*				
Solar Cells and Optoelectronics	Small-molecule crystals Annu Rev Phys Chem 66, 305 (2015)	Molecules in solution (DFT)	Absorption spectrum (~max Jsc)	yes	0.1 eV	negligible	yes
			Electronic levels (~max Voc)	yes	0.1 eV	0.1 eV	yes
			Light emission color/efficiency	limited		negligible	limited
		Small-molecule crystals (multiscale)	Crystal structure	yes	no concerns	it depends	limited
			Charge carrier mobility (~PCE)	yes	trends	large	limited
			Exciton diffusion length (~Jsc)	yes	trends	large	limited
	Conjugated polymers	Single phase (multiscale)	*Reliable modeling of semicrystalline polymers*	limited		large	very limited
	Perovskites	Single crystal (DFT)	*on target*				
Fuel Cells	*not currently in focus for theory, some calculations by MIT partners*						