Dynamic Point Defect Architectonics: Uncovering Crystal Chemical Design Rules for Tailored Chemical Expansion

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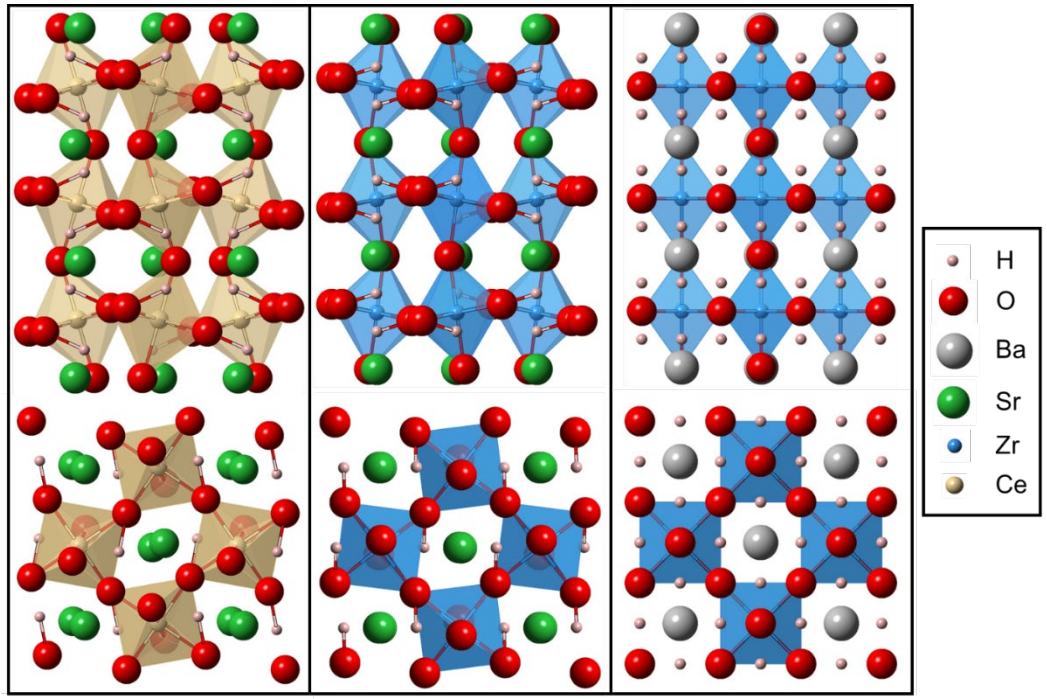
Functional ceramics strain as ions move in or out. We quantify the magnitude by the coefficient of chemical expansion (CCE), critical for electrochemical materials' stability. We develop **design principles for near-zero CCEs** based on bond architecture.

1. We studied how the **distribution of charge between anions and cations affects redox CCEs**.
- Chemical expansion trends were determined using *in-situ* dilatometry and thermogravimetry.
- Charge distribution trends and structural distortions were determined with synchrotron methods: X-ray absorption spectroscopy and X-ray diffraction.
- Redox on oxygen is beneficial for low CCEs but chemical strain anisotropy in distorted structures plays a large role too.

2. We studied how **structural distortions affect hydration CCEs**.
- Chemical expansion trends were determined using *in-situ* dilatometry and thermogravimetry.
- Atomic positions before and after hydration were determined with *in-situ* neutron diffraction (see figure).
- Intermediate distortion appears optimal for low CCEs.



Crystal structures from *in-situ* neutron diffraction vs. temperature and humidity for 3 compositions. Structural distortions increase from right to left. Our data show that the bond angles influence how ions are accommodated by the lattice and the resulting hydration coefficient of chemical expansion.

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Educational Outreach to Diverse Populations

- Delivered module for Gender Equity in Materials Science (GEMS) camp for 10th-12th graders
  - Interactive lecture/discussion on materials for electrochemical energy
  - Battery demo where students assemble different battery materials and test voltages
  - Microbial fuel cell demo where students assemble cells and observe power generation
  - Discussed week-long project posters with students and served as poster judge
- Assisted in the Franklin STEAM Academy field trip to UIUC's Materials Research Laboratory (6th-8th graders)
- Assisted in the Booker T. Washington Elementary School STEM family night

Meeting Organization

- Co-organizing "Defects and Transport" symposium at ACerS EMA conference (Feb 2024)
- Co-organizing "Mechano-Electro-Chemical Coupling" symposium at ECS Spring Meeting (2024)

Left: PI leading interactive lecture/ discussion on electrochemical energy conversion and related materials for GEMS students

Right: GEMS students assembling electrochemical cells in groups. Demo instructions are shown on screen for the students to see.