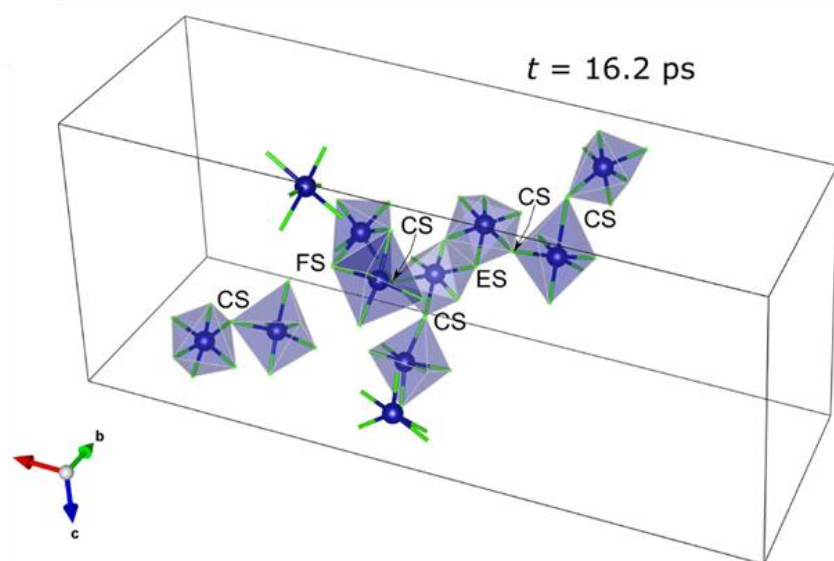


Combining X-rays & Neutrons to Study Molten Salts



The schematic depicts simulated structures showing CrCl_6 octahedra molecular chains that compose the molten NaCl-CrCl_3 molten salt (EC: edge shared, FC: face shared, and CS: corner shared). These chains were also observed in the experimental measurements.

Q.-J. Li, D.J. Sprouster, G. Zheng, J. Neufeind, A. Braatz, J. McFarlane, D. Olds, S. Lam, J. Li, and B. Khaykovich, *ACS Applied Energy Materials*, 4, 4, 3044-3056 (2021)

Scientific Achievement

Scientists determined the atomic structure of chromium (Cr)-containing molten salts & discovered a much lower melting temperature than expected, and a broad metastable liquid–solid coexistence phase.

Significance and Impact

Cr is the principal corrosion product in molten salt nuclear reactors and solar energy installation. The arrangement of ions around Cr must be determined to predict changes in molten salt properties due to corrosion.

Research Details

- Advanced neutron and x-ray scattering measurements were used in unison with molecular dynamics simulations.
- Determined temperature dependent changes in the atomic structure.
- Quantified intermediate-range order.
- Used the PDF beamline at NSLS-II for x-ray studies and the SNS for neutron studies.