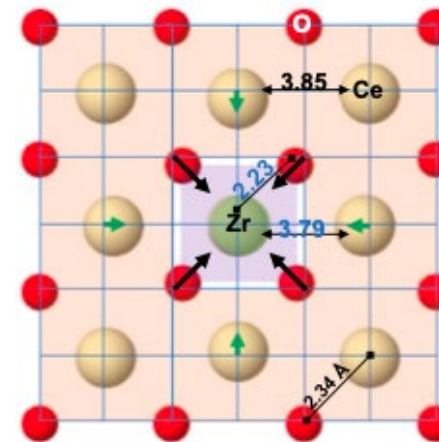
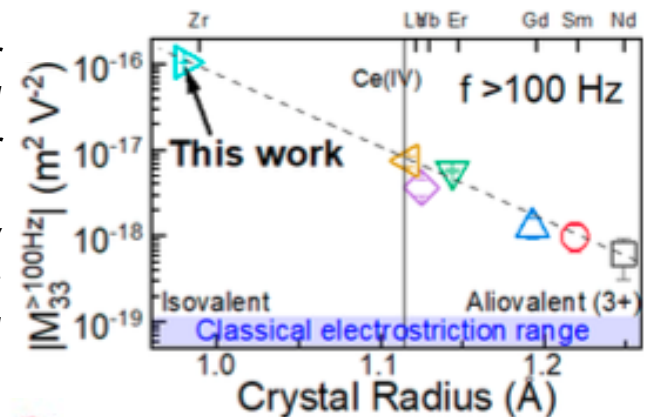


Anatoly I. Frenkel, SUNY at Stony Brook

The focus of this project is to develop fundamental understanding of processes taking place in recently discovered ceramic materials exhibiting non-classical electrostriction (NCES): low permittivity (<250) $Zr_xCe_{1-x}O_2$ with electromechanical properties rivaling those of best performing electrostrictors.

- X-ray absorption spectroscopy was combined with atomic-level modeling and electromechanical measurements to obtain the local origin of NCES: dynamic elastic dipoles.
- The elastic dipoles are produced due to the anharmonic local potential around Zr (the smaller ion) that can move freely within larger Ce-O cage.
- The dipoles are dynamic, i.e., different from the pre-existing dipoles in aliovalent doped ceria, present even without an applied electric field.
- We obtained local descriptors of NCES: the cation size mismatch and dynamic anharmonicity, that can guide future search of NCES in other polycrystalline solids.

Electrostriction strain coefficient. Data for Zr(IV) extend the trend obtained by us for trivalent dopants, hinting at a new mechanism that does not rely on pre-existing elastic dipoles



Cation-oxygen and cation-cation bond distances in Zr-doped ceria. Local structure around Zr from EXAFS analysis has Zr-O and Zr-Ce distances shorter than those for Ce-O and Ce-Ce in CeO_2 lattice, hence the free volume exists for ZrO_8 units to generate local strain.

M. Varenik, B. Xu, J. Li, E. Gaver, E. Wachtel, D. Ehre, P. Routh, S. Khodorov, A. I. Frenkel,* Y. Qi,* I. Lubomirsky.* *Nature Commun.* **14**, 7371 (2023)

Anatoly I. Frenkel, SUNY at Stony Brook**Student training**

Training of graduate students of the PI and International Collaborator (I. Lubomirsky, Weizmann Institute of Science, Israel) was strengthened by joint experiments and visits.

Interdisciplinary training by international visits

Graduate students from both institutions mentored each other: Ms. Yongchun Xiang from SBU (second from left), trained Ms. Tali Pechersky-Savich from WIS (third from left), in synchrotron data collection in December 2023. Tali trained Yongchun in materials synthesis and mechanical characterization methods.

In Summer 2023, Frenkel visited Lubomirsky's group and taught a one-day training course in synchrotron methods to a group of graduate students.



Frenkel group teamed up with Ms. Tali Pechersky (second from left), a visiting graduate student from International Collaborator, Prof. Lubomirsky's group, for synchrotron beamline measurements of Zr-doped ceria.