## MM 20: Topical Talk: Shigenobu Ogata

Time: Wednesday 9:30–10:00          Location: SCH/A251

**Topical Talk**        MM 20.1    Wed 9:30    SCH/A251
**Neural Network Atomistic Modeling of Dislocation Plasticity in Ceramics** — •Shigenobu Ogata and Shihao Zhang — The University of Osaka, Osaka, Japan

Dislocations in ceramics are increasingly recognized as levers for toughening intrinsically brittle materials and for tailoring functional responses. Yet atomistic simulation of their plasticity remains difficult because ceramic bonding combines ionic and covalent character, dislocation cores are often nonstoichiometric and charged, and core structures can be highly extended in complex lattices - features that exceed the fidelity of empirical interatomic potentials. Here, we develop neural network potentials (NNPs) for dislocation plasticity in three representative functional ceramics - ZnO, GaN, and SrTiO3. The NNPs accurately reproduce charged and nonstoichiometric core structures, slip barriers, and the long-range electrostatic interactions between charged dislocations. Leveraging these models, we examine plasticity via nanopillar compression and nano-indentation, finding excellent agreement with experimental observations. The results establish a practical workflow for constructing NNPs that enable detailed, large-scale atomistic modeling of dislocation behavior in ceramics and open new avenues for predictive exploration of plastic deformation and property tuning in functional ceramic systems.