**Global Research Outreach\_2025\_Call for Proposal**

**Theme: Semiconductor Materials**

**- Sub-Theme: New Functional Electronic Materials**

**(Computational methodology for dielectric constant prediction**

**towards the discovery of novel high dielectric constant materials)**

Multi-Layer Ceramic Capacitor (MLCC) technology continues to play a pivotal role in modern electronics, especially supporting increasingly complex circuit requirements driven by mobile devices, automotive systems, and industrial automation. Achieving greater volumetric efficiency requires continuous development of ceramic dielectrics with progressively higher effective permittivities (εeff). Thus, the discovery of entirely new, high dielectric constant (high-κ) materials surpassing the limitations of presently deployed formulations is of critical importance. Existing computational methods struggle to accurately predict these crucial dielectric properties, creating a bottleneck in the rational design process. Addressing this deficiency through innovative computational approaches is therefore imperative for sustaining technological progress. We are mostly interested in fundamental research that solve problems arising in the above areas, such as but not limited to:

* Machine Learning Accelerated Materials Prediction: Leveraging Machine Learned Potentials (MLPs) rigorously trained on high-accuracy ab initio data to facilitate high-throughput virtual screening of unexplored compositional spaces.
* First Principles Calculations Beyond DFT: Exploring methodologies transcending the limitations of Generalized Gradient Approximation (GGA)-based DFT, including Hybrid functionals (HSE06, PBE0), Many-Body Perturbation Theory (GW approximation & BSE), and Quantum Monte Carlo (QMC) calculations.
* Dielectric Tensor Calculation & Analysis: Detailed investigations into anisotropic dielectric behaviors and their relation to crystallographic orientations and internal electric fields.
* Materials Discovery & Screening: Development and application of computational workflows for systematically searching chemical and structural parameter spaces to identify promising high-κ candidates. Including database mining, combinatorial explorations, and prioritization metrics.

※ *The topics are not limited to the above examples and the participants are*

*encouraged to propose the original idea.*

※ *Funding: Up to USD 150,000 per year*