



Jianli Cheng Dissertation Defense  
NanoEngineering Ph.D. Candidate  
Yang Research Group

*“First-Principles Study of Two-Dimensional Electron Gas in  
Perovskite Oxide Heterostructures”*

*PI: Dr. Kesong Yang*

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1:30p.m.**

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**Abstract:**

Two-dimensional electron gas (2DEG) formed at the interface between two insulating perovskite oxides has provided a versatile playground to explore emergent interfacial electronic and magnetic properties. In this talk, I will talk about the electronic and structural properties of different 2DEG heterostructures (HS), with the goal of designing novel 2DEG HS using first-principles methods. In the first project, I will talk about the  $\delta$ -doping effects on the electronic and energetic properties of  $\text{LaAlO}_3/\text{SrTiO}_3$  HS with 23 transition-metal (TM) dopants. In the second project, I will talk about using high-throughput first-principles calculations and a group of combinatorial descriptors to rapidly design more than 300 novel nonpolar/nonpolar 2DEG HS. In the third project, I will introduce our newly developed software, AIMSgb, an efficient and open-source Python library for generating atomic coordinates in periodic grain boundary models. It is designed to construct various grain boundary structures from cubic and non-cubic initial configurations.