

Decoupling chemical and morphological surface defects in $\beta\text{-Ga}_2\text{O}_3$ by sum-frequency phonon spectroscopy

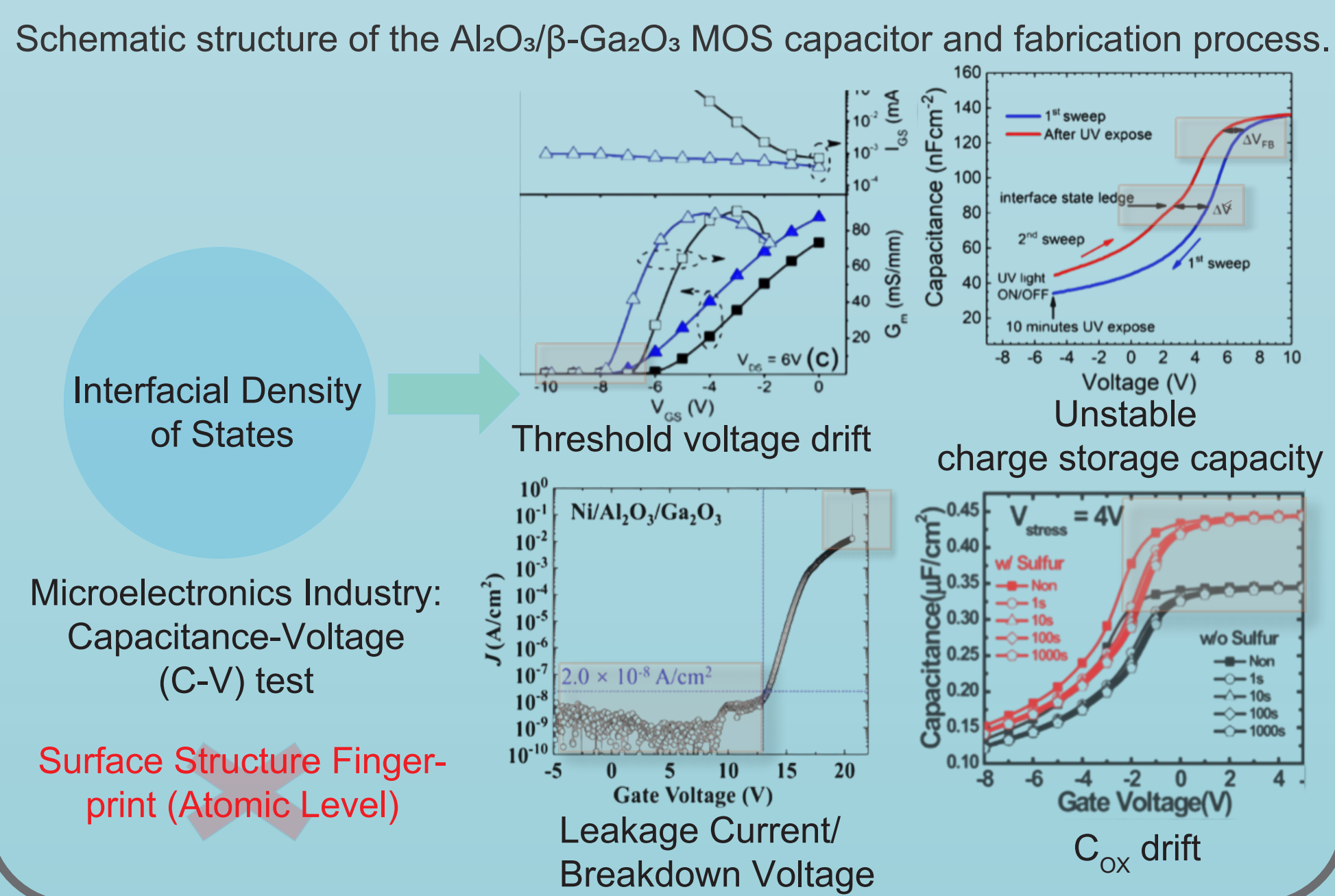
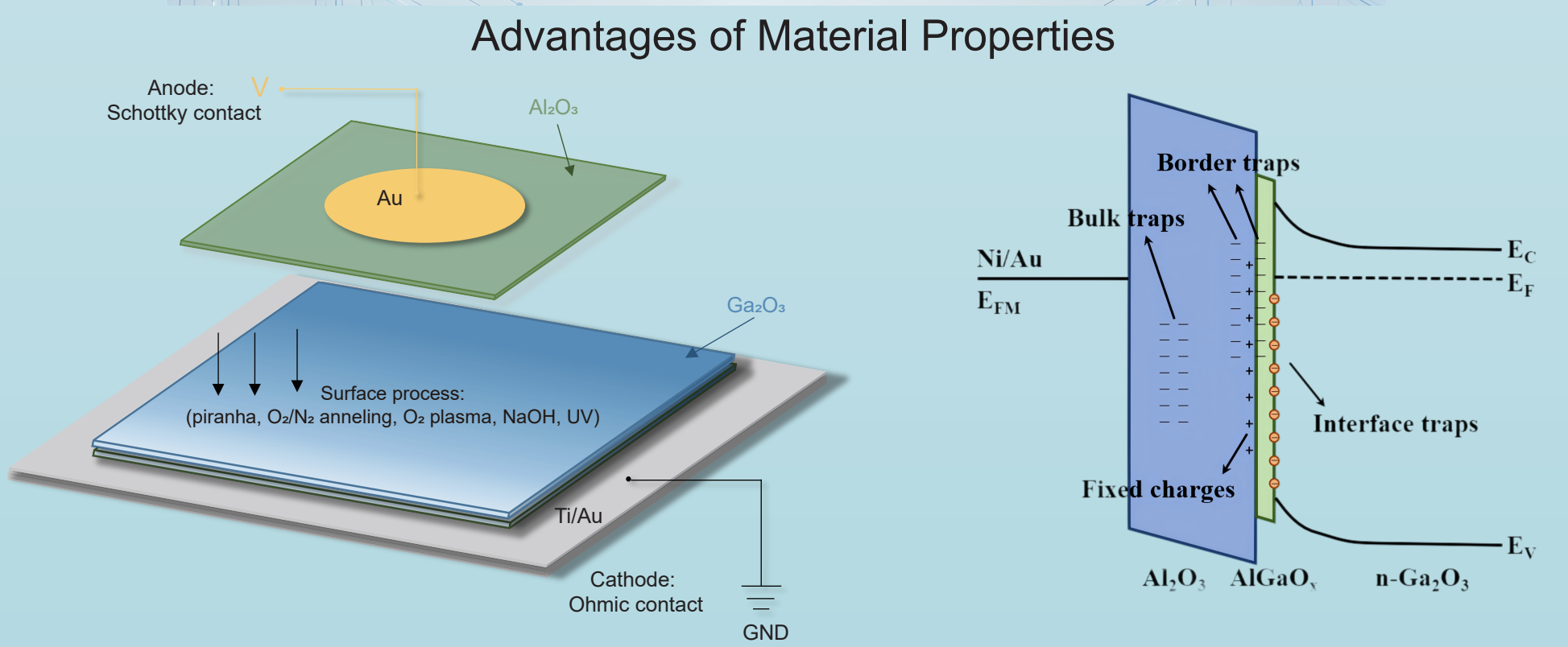
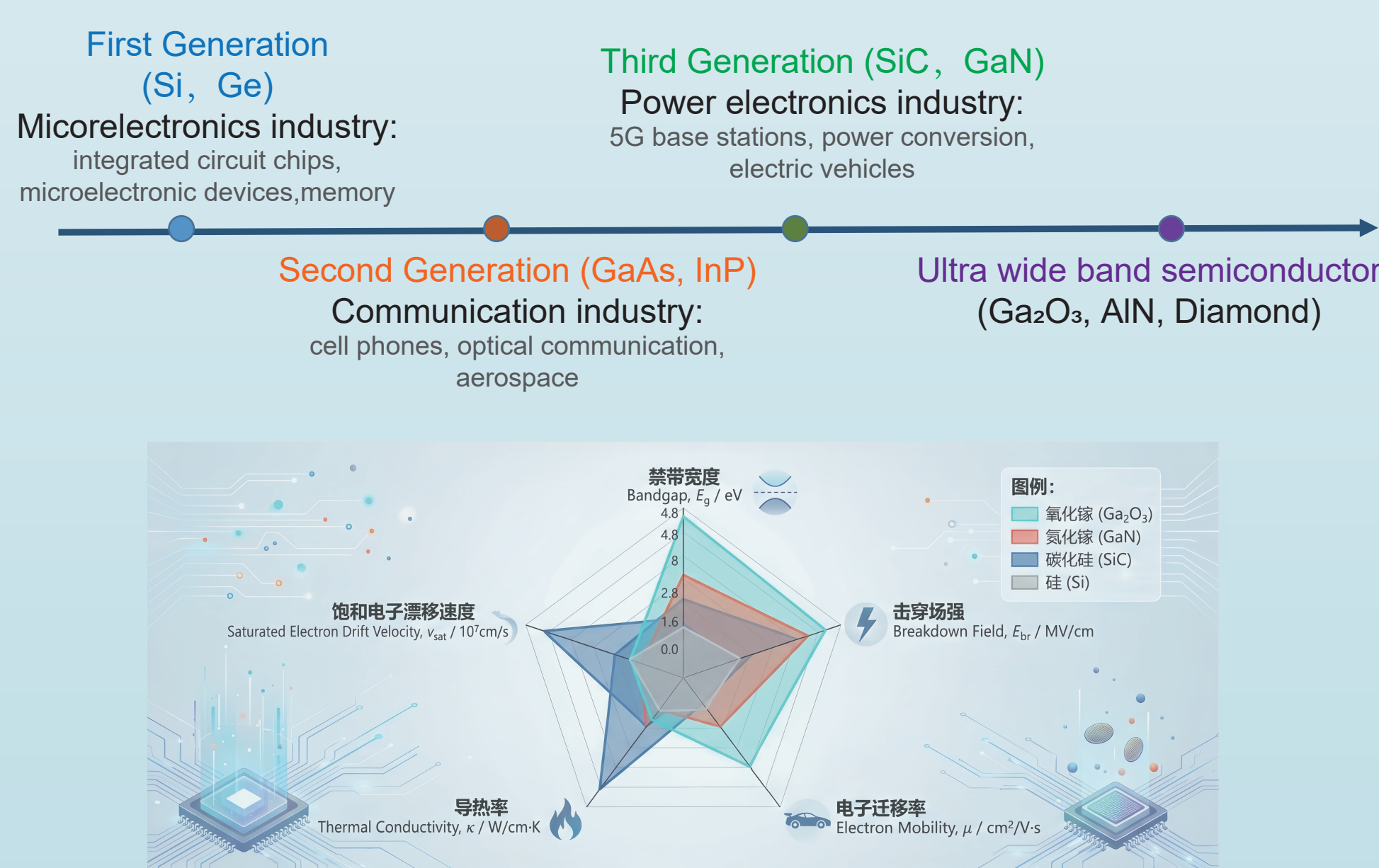
Xinyue Sheng¹, Yuxiang Lin², Xinyi Liu¹, Wei-Tao Liu^{*1}, Hao Long^{*2}

¹Physics Department, State Key Laboratory of Surface Physics, Key Laboratory of Micro and Nano Photonic Structures, Fudan University, Shanghai 200433, China
²School of Electronic Science and Engineering (National Model Microelectronics College), Xiamen University, Xiamen, Fujian, 361005, China

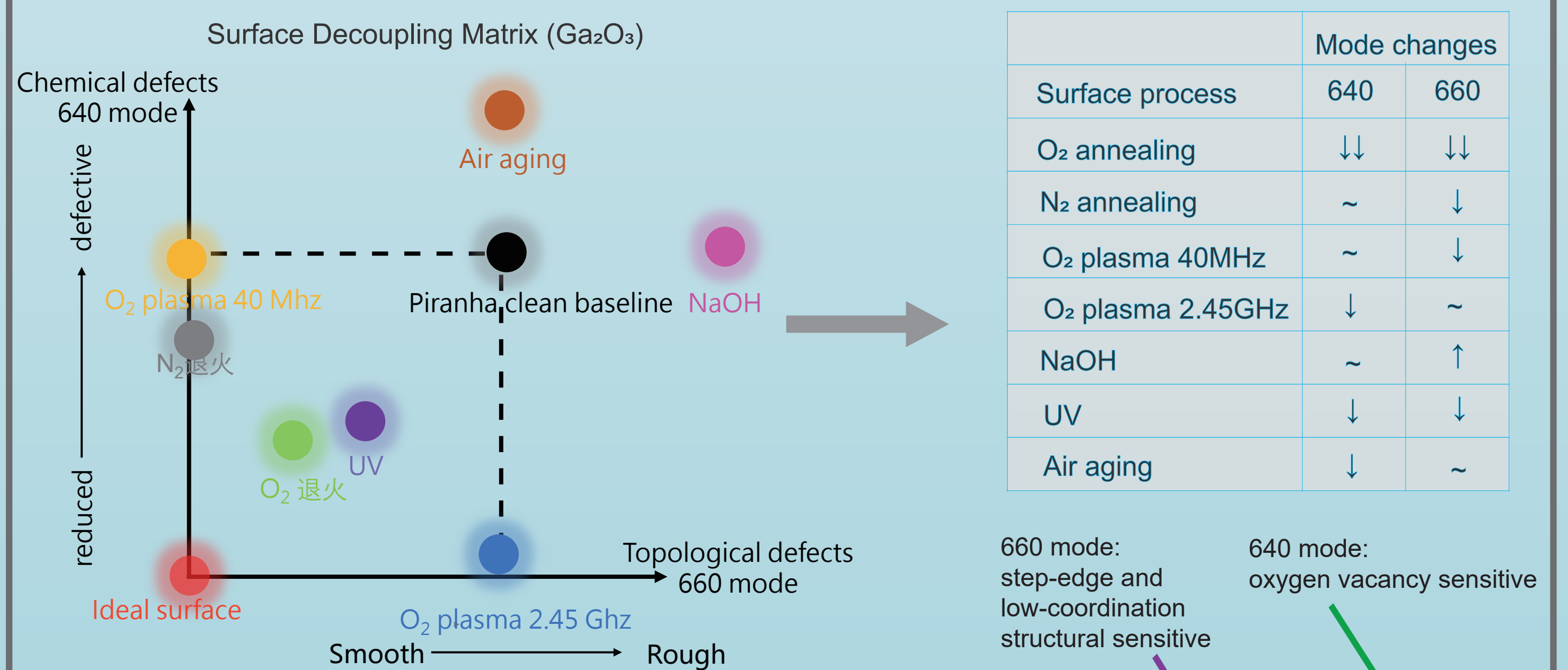
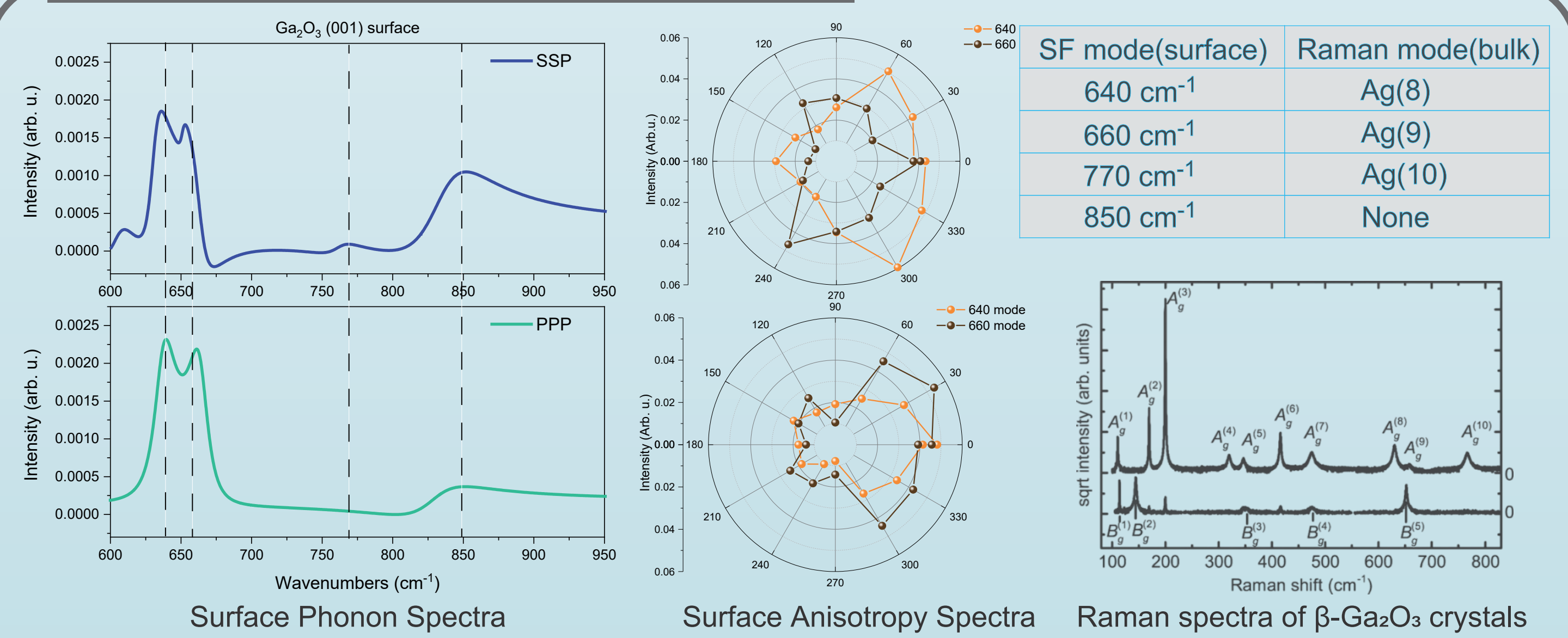
Introduction

Interfacial defect states fundamentally limit the performance and reliability of $\beta\text{-Ga}_2\text{O}_3$ ultra-wide bandgap power devices. However, traditional electrical metrology cannot resolve the precise atomistic chemical origins and topological structures of these interfacial traps. Here, we orthogonalize and decouple chemical and topological surface defects using in-situ polarization-resolved Sum Frequency Generation (SFG) spectroscopy. By rationally combining chemical etching, selective plasma treatments, and thermal annealing, we identify two distinct localized optical signatures. We assign the 640 cm^{-1} mode to Ga-O stretching vibrations perturbed by adjacent oxygen vacancies (Vo), and the 660 cm^{-1} mode to the step-edge and low-coordinated structural motifs. Furthermore, we directly correlate these microscopic probes with macroscopic device metrics: O_2 annealing completely heals Vo eliminating Fermi-level pinning and drastically reducing interface state density (Dit). Conversely, N_2 annealing induces a high-density two-dimensional electron gas verified by a hot-electron-driven continuous background. These findings provide unprecedented optical fingerprints for complex defect architectures, establishing a non-destructive atomic-scale paradigm for interface passivation in next-generation electronics.

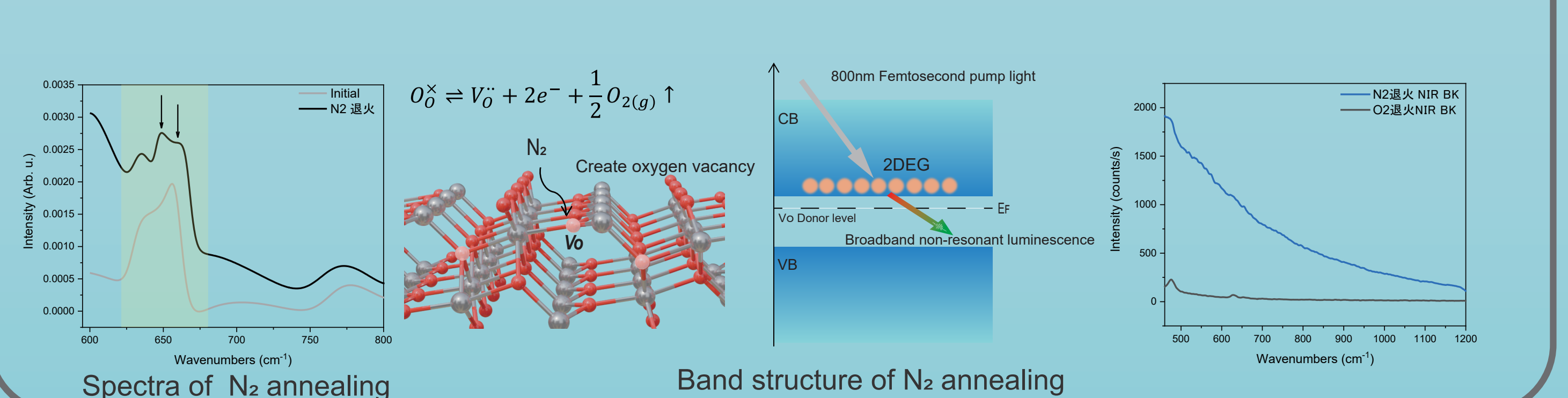
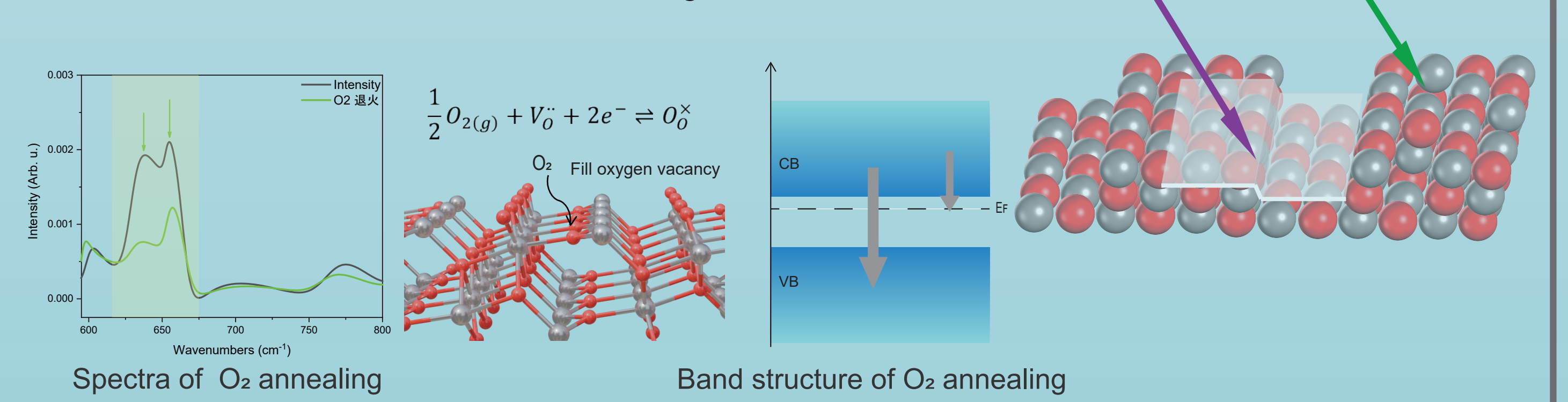
Fourth Generation— Ga_2O_3



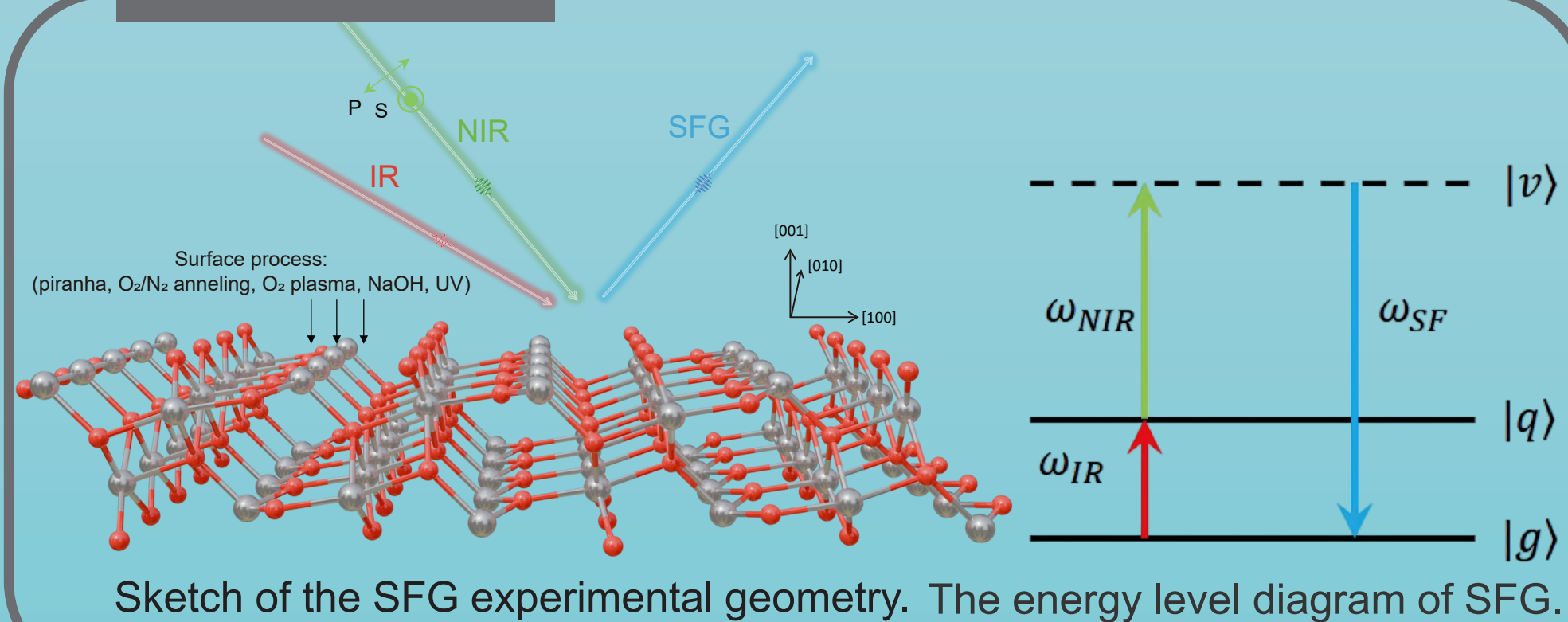
Results—Spectroscopy



	640	660
Surface process		
O_2 annealing	↓↓	↓↓
N_2 annealing	~	↓
O_2 plasma 40MHz	~	↓
O_2 plasma 2.45GHz	↓	~
NaOH	~	↑
UV	↓	↓
Air aging	↓	~



Method



Conclusion

- ◆ Orthogonal decoupling of surface chemistry and topological defects.
- ◆ Identification of 640 cm^{-1} as a chemical probe of oxygen-deficient surface environments.
- ◆ Identification of 660 cm^{-1} as a topological probe of surface structural disorder.
- ◆ Establishment of a direct correlation between microscopic spectroscopy and macroscopic device performance.

Reference

- [1] Kranert, C. et al. Sci Rep 6, 35964 (2016).
- [2] Hao Long. et al. Micrna, 208321 (2025).