Theme: Semiconductor Materials

- Sub Theme: Computational Methodology for Semiconductor Materials

The role of simulation is pivotal in the development of cutting-edge semiconductor materials that can push forward the boundaries of existing materials, by enabling the prediction of properties of novel materials that are yet to be verified through experimentation.

For the simulation of semiconductor materials, a model that can emulate chemical reactions involving surfaces (such as metals and metal oxides) and organic molecules within a periodic system is indispensable. However, the current simulation methods face challenges in accurately computing large periodic systems due to substantial costs. To overcome this hurdle, the integration of sophisticated methodologies such as advanced approximation techniques and machine learning-based approaches is deemed essential.

Therefore, we need new computational methods to analyze chemical reactions on semiconductor surfaces and materials, with the goal to circumvent the constraints of existing computational methodologies while enhancing both accuracy and efficiency.

The topics we are through this GRO are as follows:

· Fundamental and innovative simulation method for semiconductor process
· Multi-scale modeling techniques for accurate representation for metal surface and organic molecules.
· Machine learning-based approaches for surface binding. (e.g., generative AI)
· Advanced approximation methods for surface reaction. (e.g., Tight Binding).

※ *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*