Theme : Material Simulation

- Sub Theme : AI-based Retrosynthesis for Materials

Thanks to the synergy between machine learning and high-throughput computational screening, we now observe the unprecedented acceleration of materials discovery. However, we are still suffering from bottlenecks in synthesizing newly designed candidates. In this regard, we would like to assess the difficulty in materials synthesis before we walk into a lab.

We aim to find efficient and reliable AI-based *in silico* retrosynthetic design methods especially for organic semiconducting materials. And any quantitative measure for the degree of synthetic difficulty should also be deduced either from candidate synthetic pathways or from auxiliary assessment algorithms.

- For a given target product, reasonable synthetic pathways should be suggested, with or without utilizing reaction database systems. One-sided (either forward or backward) reaction prediction will not be sufficient because we usually have only target molecules at our hand.
- Since molecular complexity and synthetic complexity often differs, commercially available common materials should be considered in synthetic pathways and also in synthetic difficulty.
- Insights for *in silico* synthesis covering organometallic compounds will also be welcomed.

※ The topics are not limited to the above examples and the participants are encouraged to propose original idea.

※ Funding : Up to USD $100,000 per year