Catalysts Discovery and Understanding with Computational and Data-Driven Approaches

Youusung Jung[a]

[a] *KAIST, Daejeon, Korea*
ysjn@kaist.ac.kr
(http://qchem.kaist.ac.kr)

Novel materials discovery is a key to addressing many challenges in energy, climate change, and future sustainability. Usual procedure of finding innovative materials based mainly on experiments, however, can take far too long due to a vast and discrete search space, and thus accelerating this process by orders of magnitude using scalable computations would significantly reduce the time and cost of new discovery. In achieving this grand goal, density functional first principles simulation offers a sweet spot between the prediction accuracy and feasibility. I will demonstrate some of the examples to discover new materials in energy conversion applications using them. I will also talk about some of our recent efforts to use machine learning for chemical science that can contribute greatly to creating potential solutions to some of these materials problems.