Materials Discovery using Computational and Data-Driven Approaches

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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 storage and conversion applications using them, and also briefly describe some of our recent efforts to make density functional calculations more accurate and also scale favorably with system size. I will also talk about some of our initial efforts to use machine learning for chemical science that can contribute greatly to creating potential solutions to some materials problems.

1. Biography: Prof. Yousung Jung has received the B.S. degree from Seoul National University and Ph.D. in Theoretical Chemistry from University of California, Berkeley (2005). After a postdoctoral work at Caltech, he joined the faculty at the Graduate School of Energy, Environment, Water, and Sustainability at KAIST in 2009. His research interests involve the developments of density functional methods, and their applications for the discovery of new energy and environmental materials. He is now combining these efforts with machine learning techniques to significantly further expand the search space and achieve high prediction accuracy. He is the recipient of Pole Medal (2018, Asia-Pacific Association of Theoretical and Computational Chemists), KCS Young Physical Chemist Award under 45 (2017, Korean Chemical Society), Chemical Society of Japan Distinguished Lectureship Award (2015), and KCS-Wiley Young Chemist Award of the Year (2013).

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