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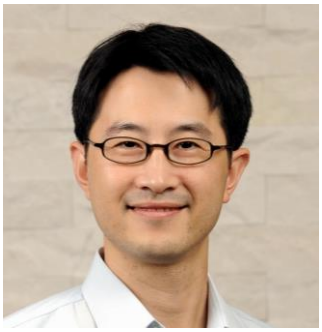
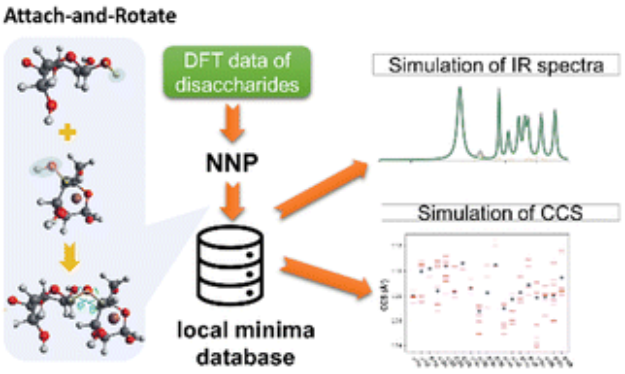


Efficient first-principles exploration on the physical and chemical space of peptides and saccharides enabled by neural network potentials

Sampling of the conformational space of peptides and saccharides with first-principles accuracy is critical as such a database provide a solid base to interpret experimental measurements such as Infrared photo-dissociation (IRPD) spectroscopy, ion mobility spectrometry (IMS), and/or collision-induced dissociation (CID). The conformational space of both peptides and saccharides are highly flexible, in which the distinct conformers of mono- and di-saccharide is estimated to be in the order of 10^3 and 10^6, respectively[1-3]. To efficiently explore the diverse conformational space of saccharide without losing accuracy, we developed a multi-level sampling scheme integrating semi-empirical models, density function theory (DFT) and neural network potential (NNP). Preliminary studies on small-size peptides with different protonated sites have also been demonstrated[4]. Solvation of these molecules can also be simulated with a computational approach that integrate fragment-based methods with NNP[5].



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