Molecular and Material Modeling Lab

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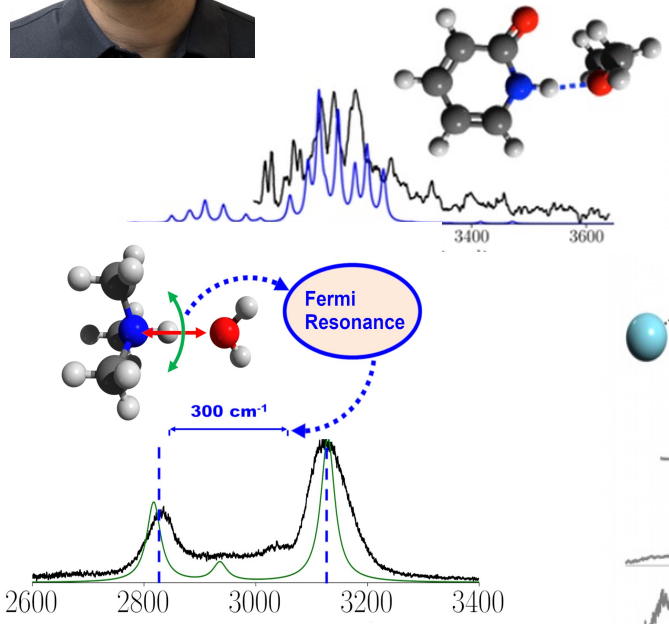
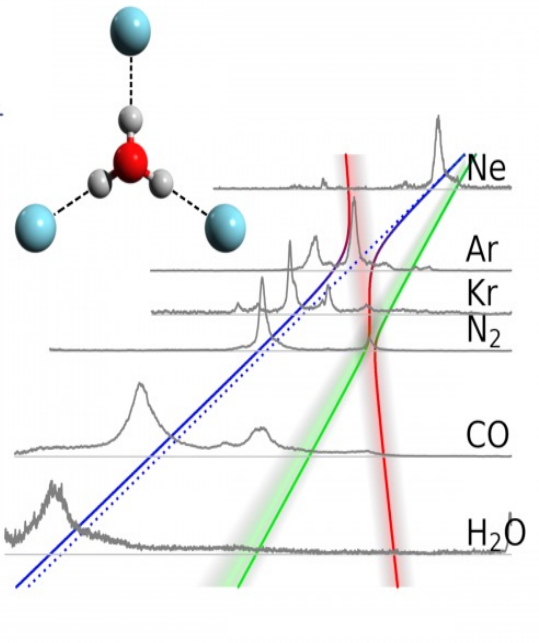
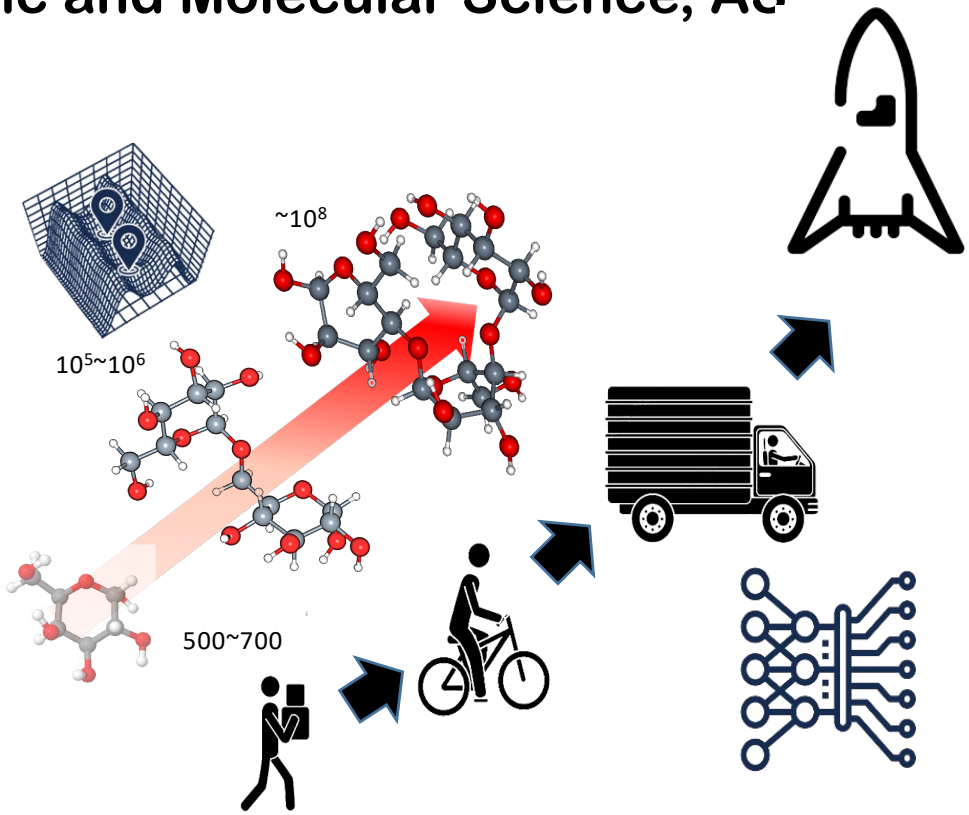


Two NH stretch in amines have very different Fermi-Resonance (FR) patterns. Our *ab initio* anharmonic algorithms (A^3) do not require empirical parameters and are able to extract simple physical pictures behind the experimental spectra and thus reduce the chance of mis-interpretation. The parameter-free reduced Hamiltonians can be use to understand physical phenomena and make predictions to guide design of experimental observations.



Complex vibrational features in experimentally observed spectra of solvated H_3O^+ lead us to understand the coupling between OH stretch and other degrees of freedom. Using *ab initio* anharmonic algorithms, we are able to assign the observed complex spectral features and to reveal simple pictures of the interplay between FR and CB in both mid- and near-IR.



We utilize deep-learning neural network potential (DL-NNP) to accelerate the exploration of energy landscape of mono-saccharides (500~1000 conformers) and di-saccharides (~10^5-10^6) with the cost comparable to semi-empirical methods & the accuracy of a decent DFT methods. We are working to improve the efficiency of sampling schemes so that we can simulate systems containing sugar, peptides and nuclear acids. We believe DL-NNP can give a boost (by several orders of magnitude) to simulations of bio-molecules that requires first-principle accuracy.