INVERSE INFRARED SPECTROSCOPY WITH BAYESIAN METHODS

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While calculating theoretical harmonic IR spectra is straightforward for most molecules, nearly all methods for incorporating anharmonic effects add a substantial computational footprint. For large systems such as molecular clusters, the brute force assignment of experimental spectra by computationally iterating over all candidate structures is infeasible at the anharmonic level. However, the developments of machine learning methods have provided an alternative route to evaluating the anharmonicities of new molecules and larger clusters, which is the subject of this talk. In this talk, we demonstrate that Bayesian optimization enables real time spectral evaluation of a range of anharmonic values applied to a calculated Hamiltonian. The Bayesian Optimization algorithm can be applied to explore anharmonic value ranges to minimize the integrated difference between the calculated and theoretical spectra. Further, this same computational framework can be adapted to assign spectra that originate from multiple isomers or cluster sizes.