GAUSSIAN PROCESSES FOR SPECTROSCOPICALLY ACCURATE POTENTIAL ENERGY SURFACES OF BENZENE DIMER

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Gaussian process regression (GPR) is a robust method for fitting functions due to the flexible ways in which covariance between calculated *ab initio* single points can be described and the relatively low amount of these training points required to achieve convergence. Increasing the complexity of the covariance (kernel) functions will systematically improve the fidelity of any given fit for functions of up to several dozen variables before the GPR becomes too computationally expensive to perform. This talk will focus on the development of a GPR algorithm to describe a 5-dimensional potential energy surface for the benzene dimer, and subsequent applications of the learned surface to spectroscopic calculations. The high symmetry of benzene allows us to decrease the number of training points even further than previously required while still maintaining faithful representation of the underlying PES. Through systematic engineering of a sufficient kernel function and both stochastic and strategic selection of training points in the conformational space of the benzene dimer, we will have access to a complete map of the necessary molecular parameters to predict accurate IR, Raman, and VSFG spectra for benzene from the gas to the condensed phase.