# Genetic Algorithms for Inorganic Oxides

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**Abstract**

Quartic force fields (QFFs) are a simple and elegant method for computing the internuclear potential term in the Watson Hamiltonian. This method is known to give agreement with experimental results between 1-5 $cm^{-1}$ for fundmental modes. Currently, there are excellent methods for performing this procedure, especially with regards to the Cartesian QFF method developed by Westbrook and Valencia that allows circumvention of the difficulty in assigning symmetry internal coordinates (SICs) for highly cyclic molecules of interest, such as polycyclic aromatic hydrocarbons (PAHs). This procedure follows the basic steps of calculating displacement energies, deriving the force constants (changes in energy with respect to displacement) using finite differences, and finally calculating the calculating the molecular vibrational frequencies by leveraging vibrational second-order pertubation theory (VPT2).

Despite this, the method is still relatively slow with calculations routinely taking weeks or longer for molecules in the order of magnitude of 10 atoms. The goal of this project is to reduce the time greatly by utilizing spectroscopic data to determine the force constants. In effect, this program reverses the final conversion from force constants to molecular vibrational frequencies. This process is non-trivial, since hundreds of variables are condensed to far fewer vibrational frequencies. A genetic algorithm (GA) is capable of performing this task.

A genetic algorithm is a metaheuristic modeled after the principles of evolution proposed by Charles Darwin. In effect, organisms have a given fitness in the environment, i.e., the problem space, and compete to pass on their "genes". In this project, an organism's fitness is an optimization solution for the minimum difference between the wanted vibrational frequencies and the organism's vibrational frequencies. Thus, the most fit organisms are more likely to pass on their genes and influence the next generation. Eventually, this population will trend towards the minimum on the problem surface, thereby yielding the force constants of interest. To date, this program has successfully calculated the force constants for water in less than 24 hours.