Project description

In this project, we aim to establish a code that allows us to optimize a set of parameters for Pt-Pt, Pt-C, and C-C pairs in the framework of the Brenner-Tersoff potential, *using machine-learnt methods*. The pair-wise potential can be expressed as:

$$V = \sum_{i}^{N-1} \sum_{j>i}^{N} f_c(r_{ij}) \left[f_r(r_{ij}) + b_{ij} f_a(r_{ij}) \right] \tag{1}$$

where r_{ij} is the inter-atomic distance, $f_c(r_{ij})$, $f_r(r_{ij})$, and $f_a(r_{ij})$ are cutoff functions,

$$f_c(r_{ij}) = \begin{cases} 1, & r_{ij} < R_{ij} \\ \frac{1}{2} - \frac{1}{2} \sin \frac{\pi}{2} \left(\frac{r_{ij} - R_{ij}}{S_{ij} - R_{ij}} \right), & R_{ij} \le r_{ij} \le S_{ij} \\ 0, & x \ge S_{ij} \end{cases} \tag{2}$$

where R_{ij} and S_{ij} are adjustable parameters.

$$f_r(r_{ij}) = A_{ij} e^{-\lambda_{ij}^{(1)} r_{ij}} \tag{3}$$

$$f_a(r_{ij}) = B_{ij} e^{-\lambda_{ij}^{(2)} r_{ij}} \tag{4}$$

where A_{ij}, B_{ij}, $\lambda_{ij}^{(1)}$, and $\lambda_{ij}^{(2)}$ are free parameters. Furthermore,

$$b_{ij} = \left(1 + \beta_{ij}^{n_{ij}} \zeta_{ij}^{n_{ij}} \right)^{-\frac{1}{2n_{ij}}} \tag{5}$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) g(\theta_{ijk}) \tag{6}$$

$$g(\theta_{ijk}) = 1 + \frac{c_{ij}^2}{d_{ij}^2} - \frac{c_{ij}^2}{d_{ij}^2 + \left(h_{ij} + \cos \theta_{ijk} \right)^2} \tag{7}$$

where β_{ij}, n_{ij}, c_{ij}, d_{ij}, and h_{ij} are independent parameters. The Brenner-Tersoff potential has already been implemented in the LAMMPS program.

The first step towards the development of this interatomic potential involves the use of a training set that constitutes a good sampling of the potential energy land- scape. In this study, we employ density functional theory (DFT) calculations to produce a training set containing (a) equations of state, (b) lattice parameters, (c) cohesive energies, and (d) elastic constants of different crystalline phases of Pt. For Pt, we consider four stable and metastable polymorphs, namely hexagonal close packed (hcp), face-centered cubic(fcc), body-centered cubic (bcc), and diamond cubic. *DFT calculations will be carried out by Dr. Bin Liu's group*.

The proposed optimization procedure can be summarized as follows (also see Figure 1):

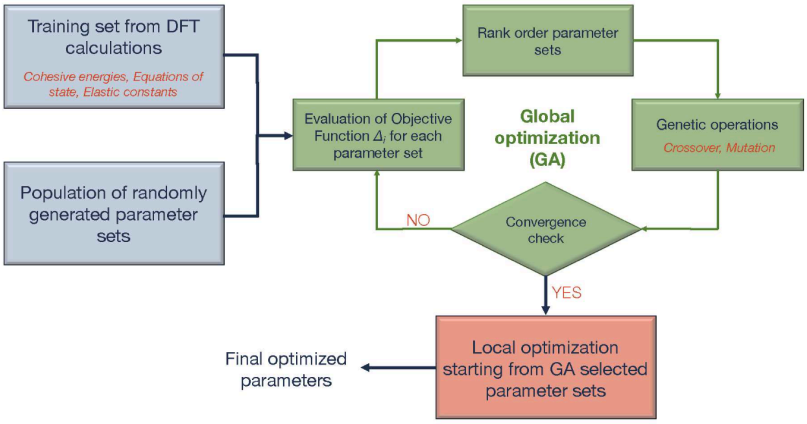

Figure 1. Schematic representation of the evolutionary strategy combining genetic algorithms and local minimization via simplex method.

1. Start with 100 parameter sets (i.e., population) that are generated randomly (Note: the initial values of these parameters are restricted within physically meaningful ranges).

2. The fitness of the objective function of a particular individual in the population is determined by a weighted sum of squared errors in its predicted properties based on the training set. The higher the objective function value, the lower its fitness will be. (Note: this can be done using the LAMMPS package, i.e., an interface with LAMMPS is needed.)

3. We select individuals (i.e., parents) using a tournament selection to perform crossover operation using simulated binary method. A fraction of the individuals are subjected to mutation via a polynomial of order 20. The probability of a crossover operation is set to 0.9. while that of mutation is 0.1.

4. Both the old and new individuals are ordered and ranked in decreasing order of their fitness. The best 100 individuals are retained for subsequent generations. This routine is repeated until the GA run does not result in any better individuals than the previous generation.

5. From the converged genetic algorithm runs, the best 20 individuals are selected for local minimization via simplex method. These 20 individuals act as starting values. The converged simplex runs are evaluated for this fitness. The one with the lowest objective function is chosen as the final optimized parameter set.