In this work, we analyze the limitations to the current approaches to the parameterization of empirical potentials. Typically, a single objective function of the weighted sum squared errors between the predictions of empirical potentials and reference targets is minimized. The choice of weights is subjective and cannot be realistically be determined *a priori.* The use of deterministic scalar optimization techniques identifies local concave solutions which are dependent upon the choice of weights and initial conditions. This process requires the constant intervention of a skilled potential developer and not amenable to an automated, algorithmic approach to potential development.

These concerns are addressed by the presentation of a novel methodology. These concerns addressed by recasting the problem as a multi-objective optimization problem where fidelity of prediction with respect to each material property is treated independently. These removes the requirement of communicating performance requirements *a priori.* The solution to parameterization expands from a single local solution to an ensemble of potentials which uses the concept of Pareto optimality. Since each potential is optimal in some sense, the potential can then be selected *a posteriori* with the performance tradeoffs between the candidate potentials.

The solution scheme for this methodology is devised, combining Monte Carlo sampling within an iterative scheme to evolution a probability distribution function representing the epistemic uncertainty of Pareto optimal parameterizations. A Bayesian-like inference process is used to periodically update the distribution function.

To automate potential development, a software library *pypospack,* is developed to automate the simulation tasks, calculate material properties, and execute sampling based optimization routines.  
  
To demonstrate the flexibility and potency of this approach, applications to specific materials systems are presented.