Tight binding parameterization through particle swarm optimization algorithm

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***Abstract*—The tight binding (TB) approach represents a good trade-off between accuracy and computational burden. For this reason, it is widely used for device simulations. However, a proper description of a physical system by means of TB requires an accurate parameterization of the Hamiltonian matrix elements (HME), that is usually done by fitting over suitable properties that can be measured or computed with first-principles approaches. We show that the particle swarm optimization algorithm is a powerful tool for the parameterization of the TB HME, using the density functional theory band dispersions of bulk reference materials as a target. We discuss the results obtained for bulk MAPbI$_3$ perovskite in its high temperature cubic phase.**

I. Introduction

Tight binding (TB) [1] is widely used for device simulations, since it allows to describe structures composed of millions of atoms, combining numerical efficiency with reasonably accurate results. In the TB approach, the wave function is expressed as a linear combination of localized atomic orbitals, that is a natural choice when we want to describe systems with atomic resolution where transport bands are formed by the interaction of atomic orbitals. However, a good representation of a physical system by means of a TB approach requires an accurate parameterization of the Hamiltonian matrix elements (HME). This is usually done by fitting over suitable properties of the system that can be measured by experiments, in this case we refer to empirical TB, or computed with more accurate approaches, such as density functional theory (DFT). Ab-initio methods based on DFT do not require adjustable input parameters to perform the simulations and offer an accurate atomistic representation of the system under investigation. Band dispersions of bulk reference materials are one of the typical targets in these fittings, useful for electronic simulations.

We propose the application of the particle swarm optimization algorithm (PSO) to the parameterization of the TB HME using the DFT band dispersion as a target. We show and discuss the results obtained for bulk MAPbI$_3$ perovskite in its high temperature cubic phase.

II. Computational Approach

The PSO was originally designed and developed by Eberhart and Kennedy [2]. In PSO, each particle is treated as a point in a D-dimensional space and explores the search area according to its own search experience and its companions' search experience. The performance of each particle is measured according to a predefined cost function f_{cost}, which is related to the problem to be solved. The i^{th} particle is represented as $x_i = (x_{i,1}, ...x_{i,d}...x_{i,D})$. The best previous position (the position giving the minimum f_{cost} value) of the i^{th} particle is recorded and represented as $p_i = (p_{i,1}, ...p_{i,d}...p_{i,D})$. The index of the best particle among all the particles in the population is represented by the symbol s. The rate of the position change (velocity) for particle i is represented as $v_i = (v_{i,1}...v_{i,d}...v_{i,D})$. The particles explore the search space according to the following equations:

$$v_{i,d} = a * v_{i,d} + b_1 * r_1(p_{i,d} - x_{i,d}) + b_2 * r_2(p_{s,d} - x_{i,d}) \quad (1)$$

$$x_{i,d} = x_{i,d} + v_{i,d} \quad (2)$$

where b_1 and b_2 are two positive constants, r_1 and r_2 are two random numbers in the range [0,1], and a is the inertia weight. Equation 1 is used to calculate the particle's new velocity according to its previous velocity (first term $a * v_{i,d}$) and the distances of its current position from its own best experience (second term $b_1 * r_1(p_{i,d} - x_{i,d})$) and the group's best experience (third term $b_2 * r_2(p_{s,d} - x_{i,d})$). Then the particle flies toward a new position according to equation 2. The inertia weight a is employed to control the balance between global (wide-ranging) and local (nearby) exploration abilities of the particles. A larger inertia weight facilitates global exploration (searching new areas) while a smaller inertia weight tends to facilitate local exploration to fine-tune the current search area.

Here, the $x_{i,d}$ positions represent the possible values of the TB HME, that determine the eigenvalues $\varepsilon^{TB}_{n,k}$ for the n band index at the k reciprocal space point. The target DFT eigenvalues $\varepsilon^{DFT}_{n,k}$ are calculated at the general gradient approximation (GGA) level, using full-relativistic projector-augmented-wave Perdew-Burke-Ernzerhof [3] pseudo-potentials. The cost function is defined as $f_{cost} = \sum_{n,k} w_{n,k}(\varepsilon^{DFT}_{n,k} - \varepsilon^{TB}_{n,k})^2$, where $w_{n,k}$ are properly determined weights.

III. Results and Discussion

We show the results obtained for bulk MAPbI$_3$ perovskite in its high temperature cubic phase. The target band structure of

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TABLE I
COST FUNCTION VALUES OBTAINED FOR DIFFERENT SETS OF THE ALGORITHM PARAMETERS a, b_1 AND b_2. IN ALL CASES, THE OPTIMIZATION IS PERFORMED USING 45 PARTICLES AND THE MAXIMUM NUMBER OF PSO ITERATIONS IS SET TO 100.

a	b_1	b_2	f_{cost}
0.1	1	1	0.39
0.3	1	1	0.13
0.5	1	1	0.035
0.5	0.5	1	0.033
0.5	1.5	1	0.034
0.5	1	0.5	0.043
0.5	1	1.5	0.031

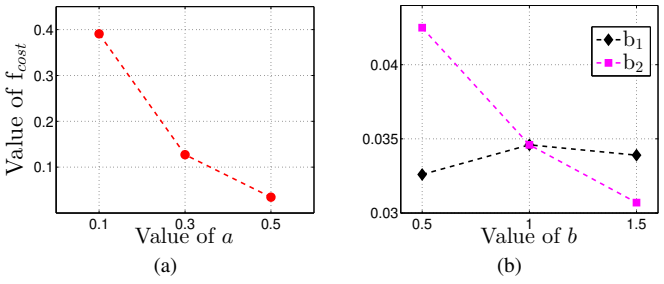

Fig. 1. Cost function values obtained for different sets of the algorithm parameters a, b_1 and b_2. In panel (a), the parameters b_1 and b_2 are set to 1. In panel (b), the parameter a is set to 0.5. In all cases, the optimization is performed using 45 particles and the maximum number of PSO iterations is set to 100.

the material is calculated at the DFT-GGA level of approximation using the QuantumEspresso package [4], adjusting the band gap energy to its experimental value [5]. The TB calculations are performed employing the TiberCAD software [6]. The choice of TB basis can be the minimal sp^3 set, as demonstrated by Boyer-Richard et al. [7]. The cost function values obtained for different sets of the algorithm parameters a, b_1 and b_2 are reported in Table I and represented in Figure 1, for clarity. It can be seen that the f_{cost} value decreases when a is increased, since the global searching is facilitated and the particles explore new areas in the search space. Moreover, when the collaboration among particles is aided (i.e., when the value of b_2 goes up) the f_{cost} value goes down. The best result is obtained for the parameters set $a = 0.5$, $b_1 = 1$, $b_2 = 1.5$. The related TB band structure is shown in Figure 2 and compared with the target DFT band structure. As an example, we show the convergence of the on-site HME for iodine p orbitals, derived with the parameters set $a = 0.5$, $b_1 = 1$, $b_2 = 1.5$, in Figure 3. It can be seen that the choice of the number of particles and of maximum iterations is sufficient to have a converged value for the HME in this case.

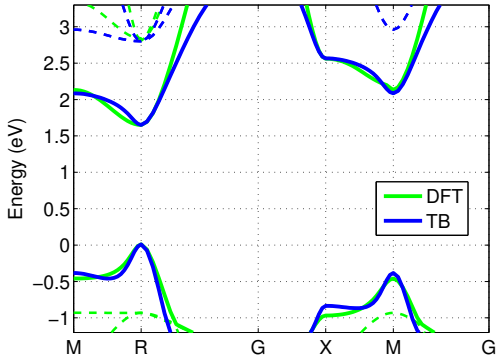

Fig. 2. TB band structure of bulk cubic $MAPbI_3$ (blue lines) derived with the parameters set $a = 0.5$, $b_1 = 1$, $b_2 = 1.5$ and compared with the target DFT band structure (green lines).

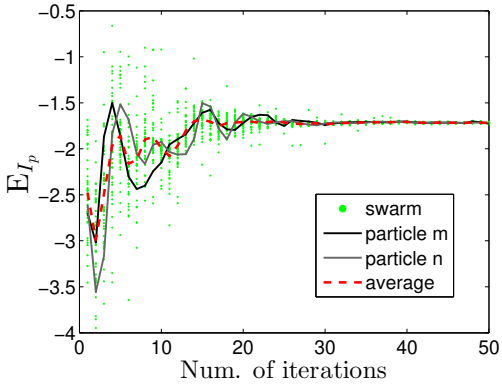

Fig. 3. Convergence of the on-site matrix element for iodine p orbitals, derived with the parameters set $a = 0.5$, $b_1 = 1$, $b_2 = 1.5$.

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