How relevant is the choice of classical potentials in finding minimal energy cluster conformations?

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ABSTRACT

We investigate the relevance of the choice of a particular classical potential in the task of finding global and local energy minima of small cluster conformations, in the context of their use as input for quantum refinement. We contrast results obtained using the many body Gupta and Sutton–Chen potentials for small nickel and copper clusters, with those of a Lennard-Jones pair potential. To obtain quantitative results we introduced a modified version of the concept of distance between configurations and color maps to represent these distances. Our main conclusion is that, for the small clusters we studied, all three potentials lead to practically the same results after quantum refinement is implemented.

1. Introduction

The search for global and local energy minima of atom cluster conformations has attracted much interest with the availability of increased computational power. On the other hand, since the physical properties of solids, liquids and clusters are mainly determined by structure, the first and crucial step in the description and understanding of condensed matter is the precise determination of the geometrical configuration that their constituent atoms do adopt [1]. Several strategies have been developed to tackle the problem, and they can be classified into three main groups: (i) finding the minimal energy structure by means of a phenomenological potential that properly describes the bulk material, and refine the global minimum thus found by quantum relaxation [2–6]; (ii) finding the global minimum plus a set of low lying local minima, followed by their quantum relaxation [7]; and (iii) perform the search quantum mechanically from the start [8,9]. Certainly, the order in which they are mentioned is related to a significant increase in computational cost. In this contribution we address several issues related to these strategies; specifically, how relevant is the choice of the phenomenological potentials used in the search for minimal energy conformations; how do the results obtained with different classical potentials compare; and, how do they match the results after quantum refinement is performed [10].

It has repeatedly been shown that the classical global minimum conformations do not necessarily correspond to the ones obtained by means of DFT calculations [6,7,10–17]. The implication is that global minima are not transferable from classical to quantum treatments. In this context several improvements have been developed, in particular Hartke [18,19] seem to have been the first to suggest a continuously adapted model potential approach to tackle the problem. This changed the way of approaching the implementation of phenomenological potentials, leading to a change of paradigm: rather than focusing on the classical global minimum we realized that the important point was to obtain a large set of local minima to be relaxed ab initio in the search of a putative global minimum among the set of resulting structures [10]. Thus, the issue of how accurate the minima generated on the basis of classical potentials have to be becomes a relevant question. In fact, when the objective is to use classically obtained minima for quantum refinement, a valid question...
seems to be if the difference between the various available phenomenological potentials does play a significant role. In this context we explore the results of the minimization process using three different potentials: two specialized embedded atom type metal potentials, Gupta type and Sutton–Chen, and a Lennard-Jones (LJ) pair potential for comparison purposes.

Actually, our aim is to determine the influence of changing the phenomenological potential on the set of local minima, a set which we denominate the configuration bank. Following a suggestion by Oganov and Valle [20], who state "The most important piece of information is the set of energy minima (including, but not restricted to, the global minimum)"; we incorporate what is expected to be a sufficient set of candidates, but not necessarily all of them, in our configuration bank. To obtain the minimum energy conformations we implement a massive application of the Fast Inertial Relaxation Engine (FIRE) algorithm, and which we denominate Massive FIRE Application (MFA). The FIRE algorithm is an efficient algorithm to determine a potential minimum, put forward by Bitzek et al. [21], who describe it as a method based on conventional molecular dynamics, with additional velocity modifications and adaptive time steps \( \Delta t \). It incorporates steering the search for the local minimum by pointing the descent along the steepest possible path, but stopping this descent as soon as the bottom of the basin is reached. Moreover, the algorithm is surprisingly fast and rather easy to implement. However, the experience we developed performing the calculations taught us that special care has to be given to the initial \( \Delta t \) value, because it strongly influences the number of force evaluations that are required, and therefore the overall computing speed of the procedure. We use FIRE because it allows to obtain a large number of low lying local minima (actually all the LJ minima for the clusters we investigate here), thus ensuring that a diverse set of low energy conformations is available. Moreover, we prefer FIRE, instead of alternatives like conjugate gradient or L-BFGS [22], because it is strictly local, it does not get stuck in transition states, and it is a very efficient procedure.

The MFA constitutes an unbiased strategy to search for the global and local minimal energy conformations of free standing nanoclusters. The objectives we seek are twofold: to find a diverse set of low lying local minima, as well as the global minimum. This way most of the local minima are found efficiently. Nevertheless, it is important to stress that our method works under stringent conditions: (i) quantum results (DFT) are assumed to be reliable; (ii) the potentials used are adequate for the elements studied; and (iii) the clusters are small.

A key point in our strategy is the proper characterization of the structure conformations, and a systematic approach to specify quantitatively their differences. To do so we modified the distance concept introduced by Grigoryan and Springborg [23]. In particular, we investigated 8, 9, 10 and 11 atom nickel and copper clusters applying all the techniques mentioned above. For larger clusters the number of minima is so large that an analysis of the sort we carry out here becomes unfeasible. In fact, for \( N = 15 \) not even the number of LJ minima is known.

This paper is organized as follows: after this Section 1 we describe our method in Section 2, where the potentials are specified, the modified distance between cluster configurations is introduced, and the details of the DFT implementation we used are specified. The results are presented in Section 3 for classical potentials, where we also test and verify the soundness of the modified distance we introduce, by applying it to copper clusters with the atoms interacting through a Lennard-Jones potential. In Section 4 we present the results obtained by means of a DFT treatment. Finally, the paper is closed by Section 5 where we summarize our results and draw conclusions.

### 2. Method

The details of the methods employed to carry out the calculations, using Gupta and Sutton–Chen embedded atom potentials, and a pair Lennard-Jones potential to compare results, the characterization and comparison of the cluster conformations, as well as the details on the DFT calculations carried out with the VASP code, are outlined below.

#### 2.1. Potentials

The procedure we use to obtain the minimal energy cluster structures is to explore one million seeds with the MFA. Three phenomenological potentials were applied to the task: Lennard-Jones [24], Gupta [25,26], and Sutton and Chen [27]. For the latter ones the parameters corresponding to copper and nickel, as given by Cleri and Rosato for the Gupta potential [25], and by Doye and Wales [28] for the Sutton–Chen potential, were employed.

The LJ potential is specified by

\[
E_{\text{LJ}} = 4\epsilon \sum_{ij} \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6
\]

where \( \epsilon \) is the potential depth, \( \sigma \) is related to the distance between atoms \( i \) and \( j \) for which the potential has a minimum, and \( r_{ij} \) is that interatomic distance. The minimal energy cluster conformations that the LJ potential yields have been widely studied and are available in the literature [29,30], and constitute a benchmark for our type of studies. The units used throughout are \( \epsilon = \sigma = 1 \). Unfortunately there is no universal phenomenological potential for metals, and therefore, while the LJ potential is certainly not universally appropriate it yields a hint on the structures, which fortunately do not differ that strongly from those obtained on the basis of Murrel–Morfram, Sutton–Chen, Gupta and Morse potentials [31].

The Gupta potential was derived to fit the cohesion energy of a bulk material [26] and is based on the tight binding second moment approximation [32]. It has two terms; an attractive part

\[
E_b = -\sum_{ij} \zeta \exp \left\{ -2q \left( \frac{r_{ij}}{r_0} \right) \right\}^{1/2}
\]

and a repulsive Born–Mayer type repulsion, which insures stability, and is given by

\[
E_r = A \sum_i \exp \left\{ -p \left( \frac{r_i}{r_0} \right) \right\}
\]

Here \( r_{ij} \) is again the distance between atoms \( i \) and \( j \), \( r_0 \) is the nearest neighbor bulk interatomic distance, and \( A, \zeta, p \) and \( q \) are the parameters that are fitted with bulk properties: the cohesive energy, the bulk modulus, and the cancellation of the energy gradient for \( r_0 \). Finally, the system cohesive energy is given by

\[
E_c = \sum_i (E_b + E_r)
\]

The values of the parameters we used for Ni and Cu clusters are given in Table 1.

The Sutton–Chen potential is based on the work of Finnis and Sinclair [33] to describe metal cohesion. These potentials are of

<table>
<thead>
<tr>
<th>Element</th>
<th>( A ) (eV)</th>
<th>( \zeta ) (eV)</th>
<th>( p )</th>
<th>( q )</th>
<th>( r_0 ) (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>0.0376</td>
<td>1.070</td>
<td>16.999</td>
<td>1.189</td>
<td>2.49</td>
</tr>
<tr>
<td>Cu</td>
<td>0.0855</td>
<td>1.224</td>
<td>10.960</td>
<td>2.278</td>
<td>2.55</td>
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</tbody>
</table>
Table 2
Parameters for the Ni and Cu Sutton–Chen potentials [28].

<table>
<thead>
<tr>
<th></th>
<th>m</th>
<th>n</th>
<th>c (Å)</th>
<th>(a) (Å)</th>
<th>(e) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>6</td>
<td>9</td>
<td>39.432</td>
<td>3.523</td>
<td>1.0</td>
</tr>
<tr>
<td>Cu</td>
<td>6</td>
<td>9</td>
<td>39.432</td>
<td>3.615</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Table 3
Number of minima obtained, for \(N\)-atom copper clusters by means of the MFA procedure \(M_{ij}\) and \(M_{cc}\) for the Lennard-Jones and Gupta potentials, respectively.

<table>
<thead>
<tr>
<th>(N)</th>
<th>(M_{ij})</th>
<th>(M_{cc})</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>8</td>
<td>7</td>
</tr>
<tr>
<td>9</td>
<td>21</td>
<td>17</td>
</tr>
<tr>
<td>10</td>
<td>64</td>
<td>34</td>
</tr>
<tr>
<td>11</td>
<td>170</td>
<td>109</td>
</tr>
</tbody>
</table>

We find that the most convenient one is the distance \(d^i(\alpha, \beta)\) defined by Grigoryan and Springborg [5], where \(\alpha\) and \(\beta\) label two particular conformations which can be obtained either with the same or different potentials, and \(i\) stands for Springborg; we use a modified version of it. Analytically \(d^i(\alpha, \beta)\) is given by

\[
d^i(\alpha, \beta) = \left[ \frac{2}{N(N-1)} \sum_{i<j} \left( d^i_{\alpha} - d^i_{\beta} \right)^2 \right]^{1/2},
\]

where \(d^i_{\alpha}\) (\(d^i_{\beta}\)) are the ordered (from smallest to largest) interatomic distances between the atoms of cluster \(\alpha\) (\(\beta\)). In fact, we used the expression given by Eq. (8) when just a single potential was employed, while slight modifications were introduced to compare conformations generated with different potentials. The expression that defines the modified distance \(d^\nu(\alpha, \beta)\), when two different potentials are used, is given by

\[
d^\nu(\alpha, \beta) = \left[ \frac{2}{N(N-1)} \sum_{i<j} \frac{d^i_{\alpha} - d^i_{\beta}}{D^\nu_{ave}} \right]^{1/2},
\]

where \(D^\nu_{ave}\) (\(D^\nu_{ave}\)) is the average bond length for cluster \(\alpha\) (\(\beta\)). It is worth remarking that while \(d^i(\alpha, \beta)\) has dimensions of length the modified distance \(d^\nu(\alpha, \beta)\) of Eq. (9) is non-dimensional, and therefore more adequate to perform comparisons. The modification introduced by Eq. (9) relative to Eq. (8) is the one that best discriminates if two clusters are equal or not, based on the experience we gained by trial and error after using several of the cluster distances available in the literature. The various average distance values \(D^\nu_{ave}\) are related to the potentials used to generate the cluster conformation. In fact, the use of Eq. (9) is equivalent to scaling the cluster sizes to make them adopt equivalent volumes, and afterward use Eq. (8) to compare their configurations.

To visualize our results when comparing cluster geometries, and since the magnitude of the values that Eqs. (8) and (9) yield has no straightforward physical interpretation, we normalize the distances \(d^\nu(\alpha, \beta)\) and \(d^\nu(\alpha, \beta)\) as follows:

\[
D_5(\alpha, \beta) = \frac{d^\nu(\alpha, \beta) - d^\nu_{\text{min}}}{d^\nu_{\text{max}} - d^\nu_{\text{min}}},
\]

\[
D_N(\alpha, \beta) = \frac{d^\nu(\alpha, \beta) - d^\nu_{\text{min}}}{d^\nu_{\text{max}} - d^\nu_{\text{min}}},
\]

where the subscripts max and min identify the largest and the smallest distance value. With this normalization \(D_5(\alpha, \beta)\) and \(D_N(\alpha, \beta)\) lie between 0 (identical to the minimum) and 1 (most

![Fig. 1](image-url)
different from it) and, as already mentioned, they are non-dimensional.

2.3. DFT calculations

In the DFT calculations we used the ab initio VASP (Vienna Ab initio Simulation Package) code [36–38] with a plane-wave basis set and GGA, using Ultra-soft pseudopotentials [39,40]. The kinetic energy cutoffs were set to the maximal default values recommended in the pseudopotential database. For the exchange–correlation functional we used the generalized gradient approximation due to Perdew and coworkers [41,42]. A cubic supercell with a side dimension of 20 Å was employed. Only the $\Gamma$ point of the Brillouin zone was evaluated, since $3 \times 3 \times 3$ Monkhorst–Pack $k$-point mesh computations, where all the atoms are allowed to relax following Hellmann–Feynman forces, yield equivalent results for the total energy. The cluster geometry is optimized, without symmetry constraints, until the total energy converges to $10^{-4}$ eV in the self-consistency loop and the force on each atom is less than 0.05 eV/Å. With these specifications we obtained for the Ni dimer an interatomic distance of 2.107 Å, a value that is close to the 2.15 Å found experimentally by Pinegar and coworkers [43]. For Cu we obtained 2.222 Å, which is in good agreement with all electron calculations in the literature, and also is in good agreement with experiment [44].

![Fig. 2.](image2.png) Representation, by means of color maps, of the normalized distance $D_N(x, \beta)$ for 8 atom local minima conformations of Cu clusters, given by Eq. (10). This renormalized distance, corresponds to the distance between the conformations of cluster $x$ and cluster $\beta$, and is symmetric respect to an axis pointing from the lower left to the top right. They are ordered in increasing energy, obtained using LJ (a) and Gupta (b) potentials. When compared with the unrenormalized distances of Fig. 1 this figure shows a better color resolution, that helps to better differentiate the various conformations. Notice that there are less minima for the Gupta than for the LJ potential. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

![Fig. 3.](image3.png) Representation by means of a color map, of the normalized distance $D_N(x, \beta)$, given by Eq. (11), between 8 atom copper clusters obtained using the Gupta and LJ potentials. $D_N(x, \beta)$ is the distance between conformation $x$ obtained using Gupta, and conformation $\beta$ obtained using the Lennard–Jones potential. Therefore, the figure is not symmetric respect to an axis pointing from the lower left to the top right, since in general $D_N(x, \beta) \neq D_N(\beta, x)$. Notice that the representation now is rectangular, illustrating the fact that the number of LJ and Gupta minima are different. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

![Fig. 4.](image4.png) Eight atom conformations of copper cluster pairs separated by the smallest distance $D_N(x, \beta)$, where $x$ and $\beta$ label Gupta (brown) and LJ (light blue) structures, respectively. Notice that $D_N(1, 2) = D_N(2, 1)$ since in general $D_N(x, \beta) = D_N(\beta, x)$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
3. Results

The first issue we want to address is to test the modified Springborg distance given by Eq. (9), and to see if we can find pairs of coincident conformations generated by the different potentials. We start by comparing the configuration banks for 8, 9, 10, and 11 atom copper clusters generated by the Gupta potential and the equivalent clusters (with the same number of atoms) generated by the LJ potential.

3.1. Copper clusters

We now present the results that we obtained. In Table 3 we summarize the number of minima obtained for each cluster size and potential used; $M_L$ ($M_G$) label the number of Lennard-Jones (Gupta) minima. The first observation that is relevant is that for the LJ potential both the number and the structure of the minimal conformations are in agreement with the literature [45,46].

The first test for the normalized distances $D_S(\alpha, \beta)$ and $D_N(\alpha, \beta)$ is to explore their behavior with conformations generated by just a single potential, and compare these results with those obtained with the original distances $d(\alpha, \beta)$. Since the amount of data we obtained is quite large we resort to colored figures to illustrate our results. We assign blue areas to clusters separated by “small” distances ($0 \leq D_S(\alpha, \beta) \leq 1$) and red to “largely” different ones ($D_S(\alpha, \beta) \geq 1$). This representation is similar to the one put forward by Mancera and Benoit [47]. In Fig. 1 we show the results for 8 atom clusters using Eq. (8), both for the LJ and Gupta potentials, where the labeling of the structures (from 1 to 8 and 1 to 7, for LJ and Gupta, respectively) corresponds to increasing energies. We notice that the LJ distances vary between $d_{\text{min}} = 0$ and $d_{\text{max}} = 0.204$ Å, while for Gupta the range is from 0 to $d_{\text{max}} = 0.404$ Å. This shows that renormalization of the interatomic distances is necessary for a meaningful comparison of clusters which are generated by different potentials.

In Fig. 2 we display a representation which is analogous to Fig. 1, but obtained using Eq. (10). This renormalized representation allows to establish a meaningful comparison between the similarities and differences of the conformations.

Once we have established that the distance defined by Grigoryan and Springborg (Eq. (8)) works properly we apply the modification put forward above, as given by Eq. (11). Comparing
the geometries generated by different potentials we can establish if
the procedure is capable of determining that the conformations ob-
tained with the Gupta potential have, or do not have, a simile in
the bank generated using LJ. To carry out the comparison we again
revert to a color map, which for \( N = 8 \) is given as Fig. 3, where
0 \( \leq D_N \leq 1 \); however, if Eq. (9) is used instead then the modified
distance values just range within the small interval between
0.003 \( \text{Å} \) and 0.138 \( \text{Å} \). With the data displayed in the color map
we are able to identify the similarity or non-equality of the geom-
etries generated by the two different potentials. \( D_N(\alpha, \beta) \) is the
distance between conformation \( \alpha \) obtained using the first potential
(in this case Gupta), and conformation \( \beta \) obtained from the second one
(in this case Lennard-Jones). Therefore, the figure is not symmetric
respect to an axis pointing from the lower left to the top right,
since in general \( D_N(\alpha, \beta) \neq D_N(\beta, \alpha) \). To further illustrate these
matters we provide, in Fig. 4, pictures of the corresponding cluster
pairs and their normalized distance \( D_N \) values.

Fig. 4 leads us to the conclusion that the modified distance
\( D_N(\alpha, \beta) \) effective and efficiently discriminates between structures,
and establishes similarities between them. Moreover, in this case \(N = 8\) we obtained 8 LJ, but only 7 Gupta, minima. Similar geometries differ mainly in the length of the interatomic distances, since the bond angles suffer only very slight variations.

We now turn to \(N = 9\) atom clusters. In this case the Gupta and LJ banks also have different number of configurations. In Fig. 5 we display the color map for the normalized distances as given by Eq. (11), where we can identify the correspondence between the geometries generated by the Gupta and LJ potentials. The pairs are illustrated in Fig. 6, where we also provide the values of \(D_N\) for each pair, and conclude that each conformation given by the Gupta potential has a LJ correspondence.

On the basis of the experience gained we next examine \(N = 10\) clusters. The color map for the normalized distances is illustrated by Fig. 7. Due to the large amount of minima we do not provide an illustration similar to Fig. 6.

Since the distance given by Eq. (11) does not discriminate between two mirror image geometries, the one in the bank will be the first one to show up in the computations. Thus, in a very large configuration bank of minimal structures we will find an equal number of “right” and “left”-handed conformations of the same energy. For our purposes we do not consider them to be different.

Finally, in order to determine if the trends outlined above persist, we study 11 atom clusters, where the number of minima is even larger. Fig. 8 illustrates, by means of a color map, the normalized distance given by Eq. (11). Unfortunately, examination of Fig. 8 provides an indication that as \(N\) grows the complexity of the situation increases considerably.

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**Fig. 12.** Comparison of the geometries of 9 atom nickel clusters, after VASP relaxation.

**Fig. 13.** DFT computed energies for 8 atom copper clusters.

**Fig. 14.** Comparison of the geometries of 8 atom copper clusters, after VASP relaxation.

**Fig. 15.** DFT computed energies for 9 atom copper clusters.
4. DFT minimization

What we learned above from small copper clusters we apply now to the DFT analysis of small copper, and also to nickel clusters. We have chosen Ni and Cu because they are straightforward to minimize quantum mechanically, which is the issue we will address next, in Sections 4.1 and 4.2. In order to compare with the first principle calculations we start providing in Table 4 the results obtained classically for 8 and 9 atom Ni and Cu clusters. \( M_L \) denotes the number of LJ minima, while \( M_E \) and \( M_{SC} \) are the Gupta and Sutton–Chen results, respectively. The Lennard-Jones minima coincide in conformation and energy with those of Doye et al. [48].

4.1. DFT approach: Ni clusters

Here we describe the first principles search of minimal energy conformations of \( N = 8 \) and \( N = 9 \) atom nickel clusters. We implemented the VASP code as specified in Section 2.3. Since the LJ minima are rather tightly packed we rescaled the distances, such that the average interatomic distance becomes \( \approx 2.86 \text{ Å} \). The DFT energies obtained using as input the minima of the LJ, Gupta and Sutton–Chen potentials, are illustrated in Fig. 9. The first thing we notice is that, independent of the classical potential used, the DFT global energy minima are practically identical. The only difference is that the Sutton–Chen structures labeled 1 and 5 yield the same energy minimum as the Gupta structure labeled 1 and the LJ structure labeled as 2. Figs. 9 and 10 also show that the LJ minima labeled as 8 yields a local minimum conformation that, while far from the global minimum, cannot be obtained using the Gupta and Sutton–Chen potentials. As far as the geometry of the global minimum is concerned our results differ from Lu et al. [48] in that the two lowest minima are interchanged, which nevertheless is in agreement with prior publications [49,50]. Our global minimum corresponds to a two layer octahedron. Moreover, we obtained all of the minima reported by Lu et al. [48], except for the cubic geometry. We again use the color coded Fig. 10 to examine our results. For example, in Fig. 10(b) we observe that the Gupta minimum for geometry 2 and the LJ for geometry 1 (and vice versa) have a normalized distance that just amounts to \( D_{NN} = 0.009 \), i.e. they are practically identical. This observation applies to all the pairs marked in dark blue.

For the \( N = 9 \) case we also had to rescale the average LJ interatomic distances to \( \approx 3.0 \text{ Å} \). The global minimum we found coincides, for the DFT structures relaxed geometries of the three potentials, with those of Nayak et al. [49], while our results differ only slightly (by 0.06 eV) from those of Lu et al. [48]. Inspection of Fig. 11 shows that the LJ, Gupta and Sutton–Chen potentials yield the same global minimum. This is corroborated by the color coded Fig. 12, where only differences between the local minima are apparent. It is also relevant to notice the asymmetry of Fig. 12, where we notice a feature that is prevalent for larger clusters, namely the dark blue areas (i.e. implying nearly equal conformations) are not necessarily along the diagonal, a feature also present when comparing different phenomenological potentials.

4.2. DFT approach: Cu clusters

We now do the same as above for 8 and 9 atom Cu clusters. Again we rescale the average LJ interatomic distance to \( \approx 2.99 \text{ Å} \), and compare with conformations obtained from Gupta and Sutton–Chen potentials. Our global minimum agrees with the literature [51–53]. It is obtained from the lowest Gupta and Sutton–Chen conformations as well as from the fifth Sutton–Chen, and the second and eight’s lowest LJ one. This is confirmed by inspection of Figs. 13 and 14.

Finally, we analyze the DFT results for 9 atom Cu clusters displayed in Figs. 15 and 16. Again it is quite apparent that all three potentials yield the same global energy minimum, as well as similar local minima conformations (dark blue areas in Fig. 16). The energy of our global minimum differs slightly (by 0.02 Ev) from the value reported in the literature [52,53].

5. Summary and conclusions

We have addressed the issue of the relevance of the choice of a particular classical potential in the task of finding global and local energy minima of cluster conformations. To do so we compared results obtained using Lennard-Jones, Gupta and Sutton–Chen potentials for nickel and copper. Moreover, we investigated if they led to different or equivalent conformations after they are used as inputs for DFT refinement. In order to obtain quantitative results we introduced a modified version of the concept of distance between configurations put forward by Grigoryan and Springborg [5], and color maps to represent these distances.

Our conclusion is that all three potentials lead to practically the same results after quantum refinement is implemented, under the proviso that: (i) quantum results (DFT) are assumed to be reliable; (ii) the potentials used are adequate for the elements studied; and (iii) the clusters are small. Consequently we conjecture, based on our results, that significant effort and computation time can be spared by just using the simple Lennard-Jones potential to generate a large set of low lying local energy minima for small clusters. Moreover, we conclude that rather than focusing on the classical...
global minimum the important point seems to be to obtain a large and diverse set of low lying local minima, and then relax them \textit{ab initio}, in the search of the putative global minimum.

Acknowledgments

Supported by the \textit{Fondo Nacional de Investigaciones Científicas y Tecnológicas} (FONDECYT, Chile) under Grants 1120399 and 1130272 (JR and MK), and \textit{Financiamiento Basal para Centros Científicos y Tecnológicos de Excelencia}.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.comptc.2013.07.004.

References