Calculation of bond length of Na-Na, Mg-Mg, and Na-Mg: A DFT study

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Abstract

*In this study, we have reported the bond length of Na-Na, Na-Mg, and Mg-Mg bu using a DFT study. In order to do it, we used a full scan to calculate bond lengths. We used 17 functional along 24 basis set. It means for each x-y consideration we have a table made of 17*24 cells. For each configuration, we reported cation, anion, and neutral bond length. At the end of the calculation, we have reported the histogram of bond length and also statistics of them.*

Keyword: *DFT,Ion Radii, Ion-Ion interaction*

Introduction

Obtaining the distance between metal ions is important in many cases. Metal ions play an important role in organic systems [1-3]. Among the metal ions, magnesium, sodium and potassium play a vital role in the activity of zygomatic cells[4,5]. Simulation of biological structures such as proteins and DNAs requires the estimation of intermolecular interactions. Since biological structures fall into the category of complex structures, it is very difficult and costly to consider the impact of the environment, considering all kinds of interactions [6,7]. Scientists in this field use some kind of statistical potential instead of physical energy [8-11]. In order to generate statistical potential, scientists need to learn a large number of predetermined structures as examples and extract statistical potential from the statistics obtained from the samples[8].

In many cases, scientists need to study a biological structure in the presence of a large number of metal ions[1]. Since there is not enough information in the database to extract the interaction of ions with each other, and it can be said with good approximation that the statistical potential calculated by the statistical data gives us a potential similar to Leonard Jones. The confusing point here is to find the minimum distance that two ions can come close to each other. This challenging issue cannot be extracted with the data in the database. Therefore, at this stage, based on the knowledge of simulation, an estimate of the distance between two metal ions should be estimated. In this paper, we have calculated the equilibrium distance between the metal ions sodium, magnesium and sodium-magnesium by using the density function method, and by applying a wider range of density functions as well as atomic base functions.

Method of simulation

In this simulation, we used GAMESS software[12]. We have the density functions HF, ROHF, LSDA, BLYP, B1B95, B3LYP, B3LYPultrafine, B3PW91, mPW1PW91, M06-2X, PBEPBE, PBEPBEultrafine, PBE1PBE, HSEh1PBE, TPSSh, BB97X-D. We also use the basic atomic functions STO-3G, 3-21G, 3-21G *, 6-31G, 6-31G *, 6-31G **, 6-31 + G **, 6-311G *, 6-311G **, 6-31G (2df, p), 6-311 + G (3df, 2p), 6-311 + G (3df, 2pd), TZVP, cc-

pVDZ, cc-pVTZ, cc-pVQZ, aug- cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ, cc-pCVDZ, cc-pCVTZ, aug-cc-pCVTZ, daug-cc-pVDZ, daug-cc-pVTZ.

This means that for each density function, we have tested all atomic base functions. Finally, equilibrium intervals are achieved by relaxing structures and minimizing energy.

Results

1. Mg-Na

To calculate the distance between two magnesium atoms, we considered three separate states of magnesium diatomic anion, magnesium diatomic and magnesium diatomic cation. Figure 1 shows the distribution of the distance between two magnesium atoms in the state of magnesium diatomic anion.

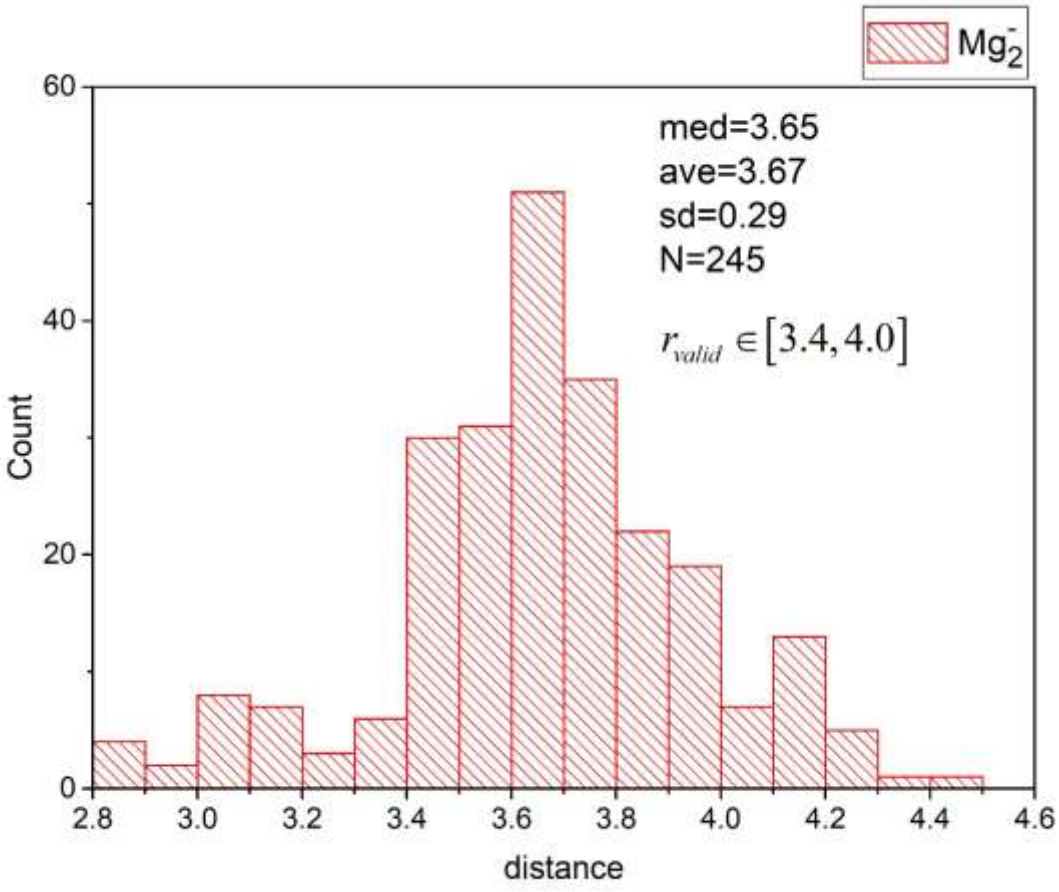

Figure 1. Histogram diagram of the distance between two magnesium atoms when they are negatively charged.

As can be seen, when two magnesium ions have a negative charge, they are on average 3.67 angstroms apart. The distance distribution is cosine and median is very close to the mean. The standard deviation is 0.29 angstroms. This means that based on DFT calculations, we suggest that when two negatively charged magnesium atoms are in the range of 3.76 ± 0.29 angstroms, they are in the bonded range, and when their distance is more than 4.0 angstroms, the energy between them is zero. If they approach more than 3.4, the energy should be positive.

In Figure 2, we examined the distance distribution of two magnesium atoms in the absence of an electric charge. This is the same as Magnesium diatomic.

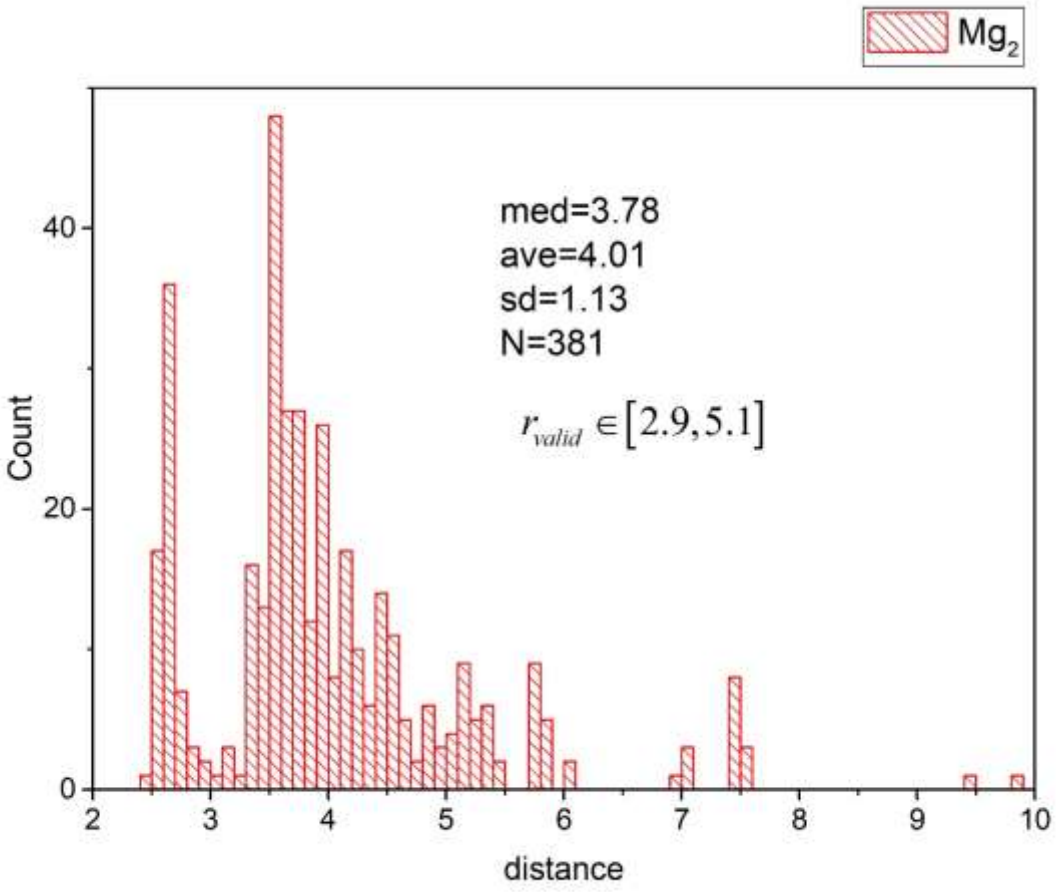

Figure 2: This graph shows the distance distribution of two neutral magnesium atoms.

As shown in Figure 2, the distance distribution is widely distributed. Median and mean are very far from each other and also deviation from the standard is a large number compared to the mean value. In this case, the average value is 4.01 Angstroms and the standard deviation is 1.13 Angstroms. It was conceivable that two magnesium atoms in the neutral state would not have a bonded Gaussian distribution.

Figure 3 illustrates the bond spacing diagram for two magnesium atoms that have a positive charge. As shown in Figure 3, there is a very strong convergence in the bonding distance between two magnesium atoms when they are positively charged. The average bond length is 2.99 angstroms. Medina is located at a distance of 3.04. The standard deviation is 0.16 angstroms. Therefore, the bond length can be defined in the range of 2.8 to 3.1 angstroms.

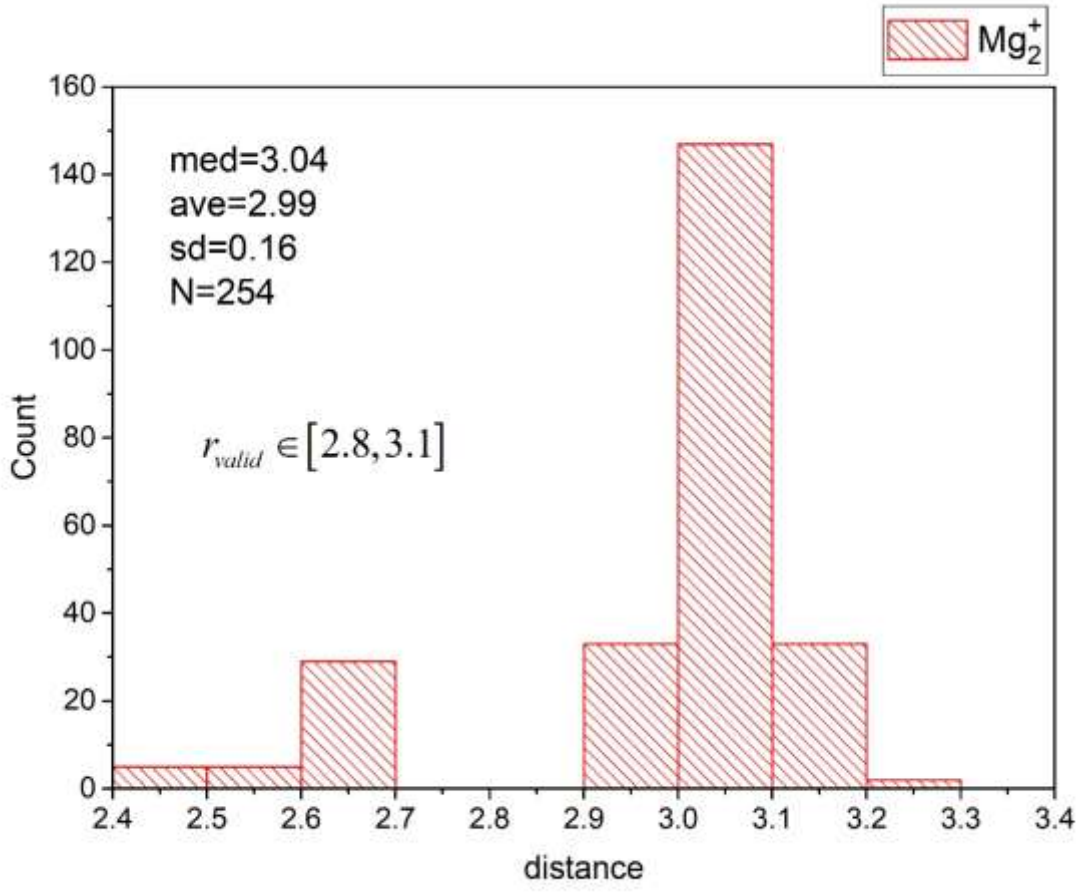

Figure 3: In this diagram, you can see the distribution of the bonding distance between two positively charged magnesium atoms.

2. Na-Na

In Table 1 you can see the bond length specifications for sodium - sodium.

	Average	Median	Standard Deviation
Na_2^-	3.56118	3.557	0.26525
Na_2	3.03413	3.077	0.21653
Na_2^+	3.60745	3.639	0.29299

Table 1: Sodium-sodium bonding characteristics

Sodium has a shorter distance in the neutral state, and when it receives an electric charge, they move slightly apart. However, as can be seen from Table 1, the standard deviation for these ions is small and the bond distance in the neutral, anion and cationic states is approximately equal.

3. Na-Mg

Sodium-magnesium does not form a stable compound when they are electrically charged, so the only data we were able to obtain was their neutral state. The two sodium-magnesium atoms have an average bond length of 4.00 angstroms and a standard deviation of 1.54 angstroms. You can see the link distribution diagram of this structure in Figure 4.

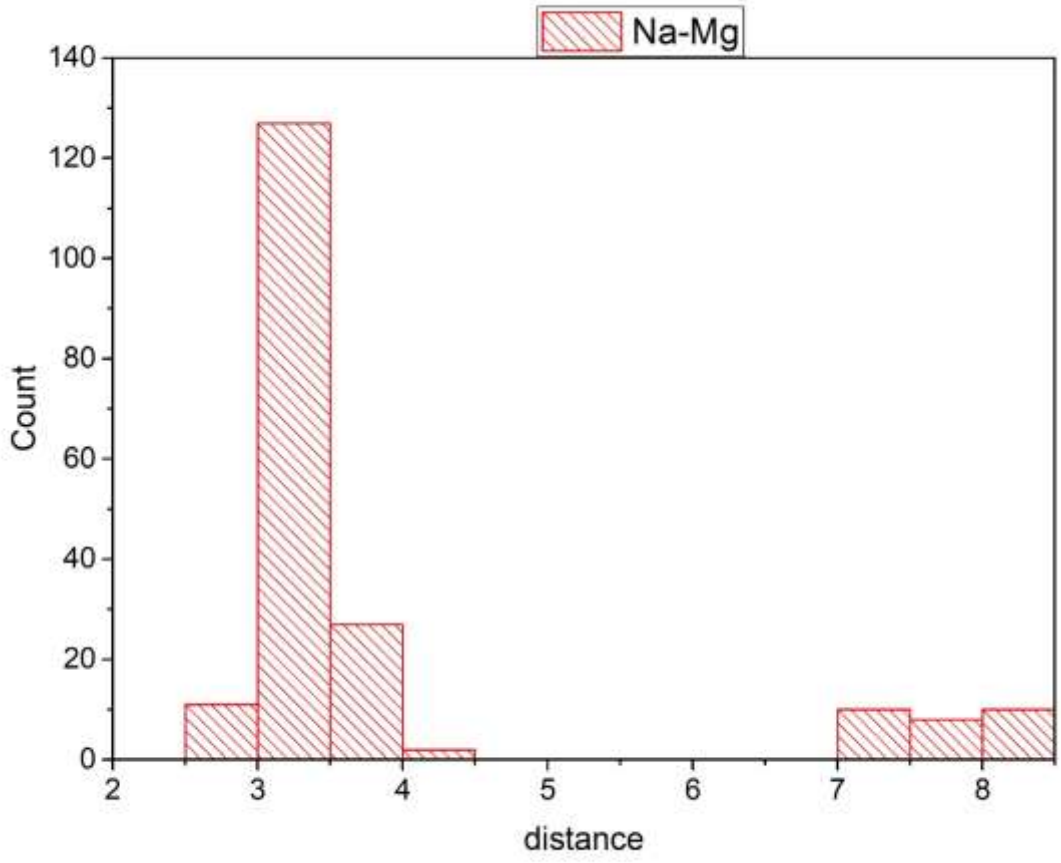

Figure 4: Graph of sodium-magnesium bonding distance

Conclusion

Magnesium in all cases tends to bind to other magnesium. However, in the neutral state, two magnesium atoms have bonded diffusion. If two magnesium atoms have a positive charge, they have the lowest bond scatter. Two sodium atoms tend to bond in all three states, and the bond length and fragmentation are similar in all three states. This is the case when sodium-magnesium bonds are formed only when the atoms are neutral.

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