Design of Orbital Based Molecular Dynamics Method

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Abstract. This paper presents a proposal of a rather new type of effective interatomic interaction for molecular dynamics and similar applications. The model consists of atoms with prescribed geometric arrangement of active orbitals, represented by arms of the length of half of the relevant bond lengths. The interactions have a repulsive part between the atomic centers and an attraction between the arm ends of different atoms. For each atom pair only the closest pair of arms interacts attempting to form the bond. This is a picture of sigma bonds, the pi bonds are modeled by alignment of additional internal vectors which might characterize a given atom. Also these are primarily pair interactions. Thus there are only pair interactions of several types present. The intrinsic arrangement of the model elements, arms and internal vectors can be switched depending on the environment. Thus the complexity of the many-body potentials is replaced by pair interactions between atoms with complex internal behaviour. The proposed model thus allows formation of new geometries, establishing new and breaking existing bonds with the use of only pair interactions and environment scanning. We discuss in some detail the carbon case and shortly also hydrogen, silicon and sulfur.
1. Introduction

This paper is concerned with a design of a rather new type of effective interatomic interaction for molecular dynamics and similar applications. A large body of empirical data is concerned with so-called bonded force fields, i.e., models where the structures in question are unbreakable but deformable, with torsion angles in addition to the stretching and compression of the bonds. The model proposed here is of the non-bonded type of interactions, also called reactive force fields, which allow formation of new geometries and establishing new and breaking existing bonds. During the last about 25 years several empirical methods were introduced to represent basic interactions between atoms, starting with the three-body interactions of Stillinger and Weber [1], several versions of the Tersoff-Brenner potentials [2], [3], the so-called Environment-dependent interaction potentials (EDIP) [4], [5], [6], and the most elaborate ReaxFF [7]. These model interactions can be used in molecular dynamics without performing any quantum mechanical calculations, they are empirical representations in some cases built on the quantum chemical studies, sometimes on models which are fitted to experimental facts. The term non-bonded models could also cover the so-called ab initio methods based on quantum mechanical approach to electronic structure, but these are generally considered separately, because their requirements and applications differ from the much simpler to implement classical potentials.

A large group of such non-bonded interactions have been extensively discussed in our paper [8], which in fact could serve as a first part of this study. This paper describes a proposal for a rather new approach to modeling the interactions between atoms which is not based on a single potential function but attempts to model explicitly the known geometrical features of bonds and orbitals. In simple terms it can be described as orbital-based interatomic interaction, which means that the dependence of the energy surface on the geometry of atomic configurations is modeled with the help of predefined orbitals. We thus wish to call the proposed model OBMD, orbital-based molecular dynamics. It will become clear that the model leads to only pair interactions. We refer also to a recent work of Rechtsman, Stillinger and Torquato [9] discussing what they called "synthetic diamond and wurtzite structures" which are self-assembled using only isotropic pair interactions as an example of special type of interactions.

Several of the existing potential models already contain features which are beyond simple potential functions, as e.g. the environment-dependent interaction potentials (EDIP) or the very detailed reactive force fields (ReaxFF). This work has been inspired also by these approaches and if the presented framework would become accepted, many empirical data could be imported from these models.

The re-orientation of the orbitals in the presented model in the MD applications would lead to the necessity to introduce some model moments of inertia and then the presence of spurious kinetic energy associated with the rotation of the atoms with respect to their
axes, which clearly does not have any physical meaning. Thus one part of the model is also a prescription to avoid this problem by introducing an over-damped rotational orientation of the orbitals, much like in the Langevin approach, but here the Langevin equations are only applied to the spurious energy which is removed by spurious friction.

In the typical potential-based applications one is using a potential with predefined parameters to simulate a physical situation. From a possible disagreement the parameters of the potential can be modified, and the aim is to model the chemistry with the basis of the chosen potential functions. Contrary to that, the proposed model aims to include as much as possible of the known chemistry by giving the atoms prototypes or blueprints of the bonds and the basic geometry as close as possible to the chemical bonds, in a way similar to the unbreakable bonds of molecular mechanics but with the built in reactivity feature, i.e. the atoms can break and form old and new bonds. At the same time the nature of the model is such that the atoms appear to interact only via two-body interactions with complex features.

The described model is not yet implemented in a full width. The parameters needed can quite directly be derived from existing model potentials, but this should be followed by comparisons and readjustments to ab initio calculations.

We start by a detailed discussion of a simple planar model in order to introduce the idea of the OBMD in section 2. The introduction and discussion of the overdamped angular motion is presented in section 3. Modeling of the carbon sheets in three dimensions relevant for graphene and graphite is the subject of section 4. Extensions needed for description of carbon structures, including the possible algorithms for implementation of the models of the structural changes are discussed in section 5. Possible applications of the proposed approach to other elements and compounds are discussed in section 6.

2. Simple planar model of the \( sp^2 \) hybridized carbon

The interaction is modelled by overlapping orbitals belonging to each atom (or what we imagine as hybridized atomic orbitals). Thus each atom looks more like a little molecule with one "heavy" atom - i.e. the actual nucleus, and the centers of the orbitals, which are located at the half length of the known bond, as a sort of additional quasiatoms. Here we think about the graphene sheet modelled by these objects with three arms. The orbitals have maximum overlap when their centers coincide - and when their axes are aligned, that is the same as when the nuclei are at the distance of the bond length and their "orbital centers" coincide.

The necessary coordinates are (in 2 dimensions)

\[
(X \ Y \ \psi)
\]  

(1)

The positions of the axes are rigid inside the atom, since we put in the model that the
ideal bond length is the property of the two neighbours. The deviation of the actual structure from the ideal bond is realized by displacing the two centers and possibly the disalignment of the arms, the arms and vertices can only be rotated.

For characterization of N-atom system are thus needed N atomic coordinates supplemented by each atom’s orientation angle (in the plane model only)

\[
(X_i, Y_i, \psi_i), \quad i = 1,...,N
\]  

where we could also use a more general vector notation \( \mathbf{R}_i = (X_i, Y_i) \) for the position vectors. On each atom the three "arms" and vertices are characterized by their positions (vectors)

\[
x_{i,\alpha} = X_i + a \cos \left( \psi_i + \frac{\alpha 2\pi}{3} \right)
\]

\[
y_{i,\alpha} = Y_i + a \sin \left( \psi_i + \frac{\alpha 2\pi}{3} \right), \quad \alpha = 1,...,3
\]  

for \( \mathbf{a}_{i,\alpha} \) of eq. 8.
or

\[ \mathbf{r}_{i,\alpha} = \mathbf{R}_i + a \mathbf{a}_{i,\alpha} \quad \alpha = 1,...,3 \]  

(4)

where \( \mathbf{a}_{i,\alpha} \) are the unit vectors of the three arms. For each pair of atoms, their nucleus-nucleus relative distance is thus

\[ r_{ij} = \sqrt{(X_i - X_j)^2 + (Y_i - Y_j)^2} \]  

(5)

and the nine distances between vertices eq. 3

\[ \rho_{i\alpha,j\beta} = \sqrt{(x_{i,\alpha} - x_{j,\beta})^2 + (y_{i,\alpha} - y_{j,\beta})^2} = |\mathbf{r}_{i,\alpha} - \mathbf{r}_{j,\beta}| \]  

(6)

which, however, are functions of only the two atomic coordinate sets eq. 2 (including the orientation angle). The distances between the vertices of i-th and j-th atom, \( \rho_{i\alpha,j\beta} \) must be accompanied by the 9 alignment parameters, or direction cosines explicitly given by

\[ \cos \theta_{i\alpha,j\beta} = \frac{1}{a^2} [(x_{i,\alpha} - X_i) (x_{j,\beta} - X_j) + (y_{i,\alpha} - Y_i) (y_{j,\beta} - Y_j)] \]  

(7)

i.e. in shorthand notation

\[ \cos \theta_{i\alpha,j\beta} = \mathbf{a}_{i,\alpha} \cdot \mathbf{a}_{j,\beta} \]  

(8)

For each pair of atoms there is thus only two-body potential, strongly repulsive between the nuclei and weakly attractive between the vertices, or orbital centers of the two atoms. That is, the nucleus-nucleus repulsion takes the form

\[ V_{ij}(r_{ij}) \]  

(9)

and the strongly coordinating nine-term potential is

\[ W_{ij} (\mathbf{R}_i, \mathbf{R}_j, \psi_i, \psi_j) = \sum_{\alpha} \sum_{\beta} w (\rho_{i\alpha,j\beta}, \cos \theta_{i\alpha,j\beta}) \]  

(10)

This all-vertex-vortex interaction is assumed only in this section, and it was the original idea of the model, which could be written as a potential.

In the present model described below, we postulate an additional saturation feature, i.e. only the pair of nearest vortices interacts, once the nearest neighbour is established, the remaining two on each atom are forgotten, they do not interact. It is a much more realistic model, only one electron from each atom is forming the covalent bond (the fact that there are so called double bonds will be discussed below).

To assure that the two vertices form a bond of the required bond length, the two arms must point against each other, other configurations must lead to higher energy.
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The simplest implementation (and thus perhaps not sufficiently flexible for all future applications) is a form of \( w(\rho, \cos \theta) \) containing a sum of an only radial term and one product term

\[
w(\rho, \cos \theta) = g(\rho) + f(\rho) t(\cos \theta)
\]

where both the radial functions \( g(\rho), f(\rho) \) and the angular function \( t(\cos \theta) \) are strongly peaked at \( \rho = 0 \) and \( \cos \theta = -1 \), respectively.

In the discussed simple planar model we find that the angular alignment can be maintained by the natural stretching resulting from the combination of the nuclear repulsion and the attraction \( g(\rho) \) of the vertices, i.e. in 2 dimensions it might be enough to consider only the first term of eq. 11 without any angular term \( t(\cos \theta) \). The above addressed feature of saturation, i.e. only one pair of vortices forms the bond, remains true also in some three dimensional cases. Thus the atom-atom interaction eq. 10 which had 9 terms reduces to one term only,

\[
W_{ij}(R_i, R_j, \psi_i, \psi_j) = w(\rho_{i<\alpha<j<\beta}, \cos \theta_{i<\alpha<j<\beta})
\]

where the two indices \( \alpha< \) on i-th atom and \( \beta< \) on j-th atom identify the pair of arms with the shortest distance between them, i.e. for all \( \alpha, \beta \)

\[ \rho_{i<\alpha<j<\beta} \leq \rho_{i<\alpha<j\beta} \]

Figure 3 demonstrates that only one pair of atoms can be attached. The third atom "learns" that the bond is occupied from the overall repulsion potential of eq. 9. The repulsive part and the attraction between the arms combine together to give a potential of the same type as all of the known interatomic potentials. For three and more atoms the attraction of the orbitals will be outweighed by the steep repulsion between atoms. In the planar geometry the alignment could be established simply by the interplay of the repulsion and attraction, without considering the angular alignment function \( t(\cos \theta) \) of eq. 11. At present we leave open the question whether this additional function is always
Figure 4. Left: The interactions of six atoms in random arrangement. Right: all ways lead to graphene structure: after the first three atoms have attached themselves (A, B, C), the next ones can only fill in gaps (D and E). See also figure B.

necessary, but clearly its presence will make the fitting of the present model generally possible to most of, if not all, the known interactions.

2.1. Example of a radial shape of the interatomic potential

It is instructive to consider the interaction energy as a function of distance between two nuclei with all the other parameters constant, when the ”arms” are kept aligned. This radial form of the potential should have a typical intermolecular potential shape. This radial form is easily obtained, it is given by the sum of the expression for the repulsion potential and the attractive potential of the two aligned arms. If the distance between the nuclei is denoted \( r \) and the length of each arm is \( a \), then the radial form of \( V(r) \) is given by

\[
V(r) = V(r) + g(|r - 2a|)
\]
where $V(r)$ is the repulsion term of eq. 9 and $g(\rho)$ is the radial part of the arm attraction potential of eq. 11.

It is quite interesting that by substituting two Gaussian shapes for both $V(r)$ and $g(\rho)$, we always obtain a reasonable shape for this fixed orientation interatomic potential of our model. For example, using $a=0.7$ Å and the following two functional shapes

$$V(r) = V_0 e^{-3x^2}$$

and

$$g(\rho) = -0.2V_0 e^{-8\rho^2}$$

we obtain the potential shown in figure 5.

3. Orientation of the bonds: overdamped motion model

The equations to be obtained from Lagrange function. Schematically:

$$\tau \ddot{\psi} = -A \dot{\psi} - \frac{\partial V}{\partial \psi}$$

(14)

where $\tau$ is a fictitious moment of inertia of the atom and $A$ is also fictitious coefficient of ”angular friction”. These two parameters would be needed in the model to assure a reasonable behaviour of the simulations. A method which avoids this additional complexity is to assume that the angular motion is ”overdamped”, analogous to the over-damped Langevin motion. This means that

$$-A \dot{\psi} \gg \tau \ddot{\psi}$$

where $A$ must be adjusted (as a free parameter) and instead of the second order equation the angles are updated according to

$$\dot{\psi} = -\frac{1}{A} \frac{\partial V}{\partial \psi}$$

(15)

4. The graphene sheet model in three dimensions

In this section we discuss the extension of the previous model to 3 dimensions. The model is extended by the rotation axis of each atom, perpendicular to the plane where $\psi$ is measured. The unit vector is given by the two customary angles $\theta$ and $\phi$. The model thus consists of atoms which contain three arms as in previous section and in addition a specified direction vector $n$ which is perpendicular to the plane of the arms. The variables describing the atom are thus the arms as in previous section and the additional direction vector, specified by the two angles (analogy to the Euler angles).
For characterization of N-atom system are thus needed N atomic coordinates $\mathbf{R}$ supplemented by each atom’s three orientation angles $\theta$, $\varphi$ and $\psi$

$$(\mathbf{R}_i, \theta_i, \varphi_i, \psi_i), \quad i = 1, \ldots, N$$

where $\psi$ as before specifies the rotation of the arms while the angles $\theta$ and $\varphi$ specify the normal to the plane of the arms, as well as the rotational axis for the rotation by $\psi$. Note that we adopt a notation where

$$\mathbf{n}_i = (\sin \theta_i \cos \varphi_i, \sin \theta_i \sin \varphi_i, \cos \theta_i)$$

The interaction between the arms is identical to the previous section, a new element added is the simulation of the $\pi$-bonding by pairwise alignment of the axes of the interacting atoms.

The nature of the $\pi$-bonding does not require the saturation feature discussed above, rather the requirement that the two atoms engaging in this new interaction also already interact via one of the arms-pairs. There are now three angular variables instead of one and the equations for angular motion become more complex. The generalized gradient and torque will update the angles again through first order equations, since the model assumption of over-damped motion is also present here.

Formally, the interaction can now be written as follows. The atom-atom interaction analogous to eq. [10] becomes now

$$W_{ij}^{\pi}(\mathbf{R}_i, \mathbf{n}_i, \psi_i, \mathbf{R}_j, \mathbf{n}_j, \psi_j) = w (\rho_{i\alpha<j\beta<}, \cos \theta_{i\alpha<j\beta<}) + g \left( |\mathbf{n}_i^\perp \cdot \mathbf{n}_j^\perp| - 1 \right)$$

where the two indices $\alpha<, \beta<$ on i-th atom and $\beta<, \gamma<$ on j-th atom are given by the minimal distance between them (the pair out of the nine with the shortest distance),

$$\rho_{i\alpha<j\beta<} \leq \rho_{i\alpha,j\beta}$$

for all $\alpha$, $\beta$ and the $\theta_{i\alpha<j\beta<}$ is the angle between these two arms - this time in the full three-dimensional space. The vectors $\mathbf{n}_i^\perp$ and $\mathbf{n}_j^\perp$ are the components of the vectors $\mathbf{n}_i$ and $\mathbf{n}_j$, perpendicular to the line connecting the two atoms,

$$\mathbf{n}_i^\perp \cdot \mathbf{r}_{ij} = 0 \quad \mathbf{n}_j^\perp \cdot \mathbf{r}_{ij} = 0$$

It should be noted that the term

$$g \left( |\mathbf{n}_i^\perp \cdot \mathbf{n}_j^\perp| - 1 \right)$$

is a new model effective interaction which can be understood as related to a part of the dipole-dipole interaction (cf. [10]),

$$\mathbf{n}_i^\perp \cdot \mathbf{n}_j^\perp - 2 \mathbf{n}_i^\parallel \cdot \mathbf{n}_j^\parallel$$
Figure 6. Representation of the so called sp²-hybridized orbitals of a carbon atom

Figure 7. Schematic drawing of a group of carbon atoms with sp²-hybridized orbitals forming a part of the planar graphene structure.

namely the part which would describe the attraction of two small magnets when they are oriented antiparallel to each other and perpendicular to their connecting line. We discuss this particular feature and this model mechanism of sheet alignment in more detail in a short paper [11] where also results of a small simulation demonstrate that this model interaction really leads to planar alignment. We add that the neglected part of the dipole-dipole expression above, i.e. for the vectors aligned with their connecting line, can be used to position at the desired distances of the different sheets. Thus the representation of graphite situation can be based on split and re-shaped dipole-dipole type interaction where the transverse term aligns each sheet while the parallel term has such radial dependence with a minimum at the known distance between sheets of graphite.

5. The Carbon Story

A group of carbon atoms will interact in many different ways, depending on their mutual relations. Up to now we have discussed the situation known as sp²-hybridization of atomic orbitals. In this section we will try to extend this to the other known situations. The discussed models should describe all known carbon relations to other carbon and hydrogen atoms, including the two diamond structures.
5.1. Formation of carbon strings

The free carbon atom in this model looks as shown in figure 8. It is not really a free

\[ R_s^2, R_p^2, R_\perp \]

\[ \sigma_1, \pi_1, \pi_2 \]

\[ \text{Figure 8. Representation of the so called sp-hybridized orbitals of a carbon atom} \]

atom, which should have electron configuration $2s^2 2p^2$, but it reflects the fact that a

smallest stray electric field would lead to Stark states in some direction, which then

would become the two $\sigma$ states, represented by the two arms (with centers of future $\sigma$

bonds denoted by small circles). The two (perpendicular) $\pi$ states are shown by the two

transverse lines perpendicular to the $\sigma$ states and to each other.

The formula for atom-atom interaction in this case is a simple modification of eq. 17

\[ W_{ij}^s (R_i, n_i, \psi_i, R_j, n_j, \psi_j) = w (\rho_{i\alpha<j\beta<}, \cos \theta_{i\alpha<j\beta<}) + \sum_{\mu\nu} g (|n_{i\mu}^\perp \cdot n_{j\nu}^\perp| - 1) \]

where $\alpha<$ and $\beta<$ have the same meaning as in eq. 17 while the sum runs over the

representatives $\mu, \nu$ of the two $\pi$-orbitals on each atom. The emerging carbon strings

are referred to as carbyne, and there have been some discussions about its forms with

alternating single and triple bonds in contrast to equivalent double bonds in a chain.

It should be noted that the presented model can not distinguish the two alternatives

unless some further features would be added.

5.2. Graphene and graphite.

In a situation when there are more than two close neighbours, it will become energetically

advantageous to have more electron-orbital mixing than just one Stark mixture, which

can lead to the formation of additional sigma orbitals (bonds) with neighbour mixture.

This would switch the atom’s behaviour from $sp$ hybridization to the $sp^2$ hybridization

shown in figure 6 with the interaction form already described by eq. 17.

In figure 8 is shown how the $sp^2$ hybridized states lead to formation of the planar carbon

structures.

The $\pi$-orbitals on all atoms prefer to be aligned, this reflects the formation of $\pi$-bonds

and in fact also the origin of the $\pi$-type electronic energy bands in benzene and in
particular graphene. The correlation over many atoms of the $\pi$-type bands has an important energetic effect and this could be built in a future version of the proposed model. For the time being we only consider the alignment of the $\pi$-vectors.

5.3. Diamond-like structures

When there are more than three neighbours, the energetic advantage leads to $sp^3$ hybridization and geometry shown in figure 9 i.e. there are no orbitals left in the pure $\pi$-form, all four orbitals lead to formation of $\sigma$-bonds.

$$W_{ij}^{t} (\mathbf{R}_i, \mathbf{n}_i, \psi_i, \mathbf{R}_j, \mathbf{n}_j, \psi_j) = w \left( \rho_{i\alpha<j\beta<}, \cos \theta_{i\alpha<j\beta<} \right)$$ (19)

where $\alpha<\beta$ have the same meaning as in eq. 17 but in this case the minimal distance is chosen from the possible 16 instead of 9 pairs. Note that now there is no dipole-type interaction included.

Interaction of tetrahedral $sp^3$-atoms would lead to the chain formation of aliphatic hydrocarbons in combination with sufficient hydrogen - or to the mesh of carbon layers of diamond-like and lonsdaleite-like type structures.
The basic three-atom group is sketched in figure 10. This three-atom group appears both in diamond, lonsdaleite and in hydrocarbons. The bond lengths will be different in different situations, in our model the arm lengths are set up by each atom depending on its "knowledge" of the neighbourhood. This shows the flexibility of the proposed approach. One can put in various instructions for changing the atomic parameters depending on the environment, i.e. every atom is a sort of automaton with instruction set allowing to enter as much chemistry as desirable.

One of the situations which can be used to adjust the interaction parameters is represented by figure 11 where the hydrogen nucleus is the simple vertex, a line with atom at the end, and where the center of the sigma orbital is shown by the circle as in the other diagrams, i.e. the molecule of propane.

5.4. Four body correlations in diamond and lonsdaleite.

In our previous work we discussed how to include the four-body correlations into the Tersoff-type and Stillinger-Weber type models. Here we describe another feature added to the present model which will make it possible to energetically differentiate diamond from lonsdaleite, i.e. build in an effective four body correlation using the interaction form of two-body forces of the type introduced in this paper.

The two different types of planar carbon chains present in diamond and lonsdaleite are shown in figure 12. The chain (a) is already shown in figures 10 and 11, and it is present in both diamond and lonsdaleite, while the chain (b) is present only in lonsdaleite. We shall now construct an effective interaction leading to the alignment of structures of the type (a). Comparing the two structures, it is easy to see (especially when using a three-dimensional molecular modeling set) that the chains of figure 12 are repeated in three planes which have in common the line connecting the two atoms, i.e. one pair of the "arms". In the case (a) the three unconnected "arms" on each of the neighbor atoms point in exactly opposite directions, it means that in the case (a) all four pairs of the arm vectors directionally closest (lying along the same line, but in opposite sense)
to each other are having scalar products equal to $-1$. In case (b), and in any other conformation of carbon or aliphatic hydrocarbons, this is never the case. The desired effective interaction can be described by a spin-spin type formula

$$U_{ij} = u(r_{ij}) \sum_{\alpha\beta} |\mathbf{a}_{i\alpha} \cdot \mathbf{a}_{j\beta} + 1|$$

(20)

where $\mathbf{a}_{i\alpha}$ are the unit vectors of the "arms" and the summation runs only over the four pairs of the total 16 which are directionally closest, i.e. give the smallest contributions. This formula will give zero for the diamond arrangement and a positive energy penalty for any other orientation of the two model atoms. When additional atoms are added to the ends of the discussed "arms", this two-body interaction results in four-body correlations.

5.5. Environment dependent switching of interactions

An essential feature of the proposed model is the switching of a given atom’s behaviour between the $sp^2$ to $sp^1$ or the $sp^3$ regimes. In the EDIP model this is implemented by adding a more or less continuous function. Here we propose a sort quantum jump switching behaviour. However, it does not mean that the structure will change by a jump. Only the relation of the arms (and in fact their number, only the $\sigma$-orbitals are represented by arms) If an atom can not find and get aligned with two perpendicular $\pi$-vectors, it will switch from the $sp^1$-regime of figure 8 to the $sp^2$ regime of figure 6.

The conditions for the switching and their implementation are the strength of the proposed model, but on the other hand they represent a problem since at present we do not yet have a realistic prescription. This must be obtained both from chemical observations and from quantum chemical calculations.

When considering the $sp^3$-regime, we should mention the representation of hydrogen
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atoms, which simply are one-armed atoms with a suitable arm length to complement the length of the carbon arm so that their sum becomes the length of the hydrogen to carbon bond.

6. The Silicon and Sulfur Story

The situation for silicon which has four valence $n = 3$ electrons is quite different from the carbon case of $n = 2$ electrons. Si-atoms would not experience the $sp^2$-hybridization of atomic orbitals which is so important for carbon, i.e. clearly no $\pi$-bonding in addition to the $sp^3$-hybridization of atomic orbitals. On the other hand, groups of Si atoms can arrange themselves in many other geometries (at higher temperatures). The proposed model could be used in place of the Tersoff potential for situations where the diamond-like structure remains the most important feature. For description of these cases the present model concentrating mainly on the features seen for $n = 2$ atomic states should be extended to model also further features of higher atomic states.

Oxygen and sulfur are another pair of similarly related elements with $n = 2$ and $n = 3$ orbitals, respectively. These elements show even more different behavior than carbon and silicon. In particular the complex behaviour of sulfur aggregates presents a problem not well studied in the framework of simple models. Extensions of the present model to many such new situations do not seem to be hindered by anything else than suitable representations of further features, derived from known chemical observations. In particular, the known complexity of sulfur behaviour including the $S_8$ rings (cf the work of Stillinger and Weber on liquid sulfur [12]) might be well modelled with the help of future extensions to the discussed model.

7. Conclusion

We have formulated a procedure for a design of a model empirical atomic interaction which has the ability to incorporate many more features than the traditional two- or three-body potentials. These many feature are directly connected with observed facts, since the interactions are pair interactions only. This is made possible by basing the model on predefined orbitals, much like the molecular structure models invented by Andre Dreiding. A natural name for the model would thus be the Dreiding interactions, but unfortunately the Dreiding force field already exists and does not have any of the features discussed here. We have thus chosen the name OBMD for the proposed approach.

The model is not yet practically implemented, we hope that we shall attract experts on different aspects to contribute to the fitting and modeling of the details. In concluding, we show how powerful the idea is by simply considering the possible shapes
of the potentials. In the traditional potentials, there are usually present two different inverse powers with opposite sign (Lennard-Jones type), or two exponentials of different exponent (Morse type, Tersoff etc), in our approach we can combine even two Gaussians to obtain a nice shape for the potential as shown in figure 5. This is naturally made possible by the fact that the two gaussians are not centered at the same point, but one at the atomic center and the other at the orbital center.

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