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Development of the orbital-free approach for hetero-atomic systems

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The key problem of the orbital-free approach is calculation of kinetic energy, especially for hetero-atomic systems. In this work, we used the mono-atomic functionals of kinetic energy to construct the kinetic functionals of complicated systems. We constructed some atomic weights associated with densities of single atoms and then calculated kinetic functions for some atomic complexes. For the examples of SiC, SiAl, AlC, SiO and CO dimers we have demonstrated possibility of our approach to find equilibrium interatomic distances and dissociation energies for hetero-atomic systems.

Keywords: orbital-free, density functional, hetero-atomic systems, interatomic distances, dissociation energies.

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1. Introduction

Nanotechnology requires simulation methods, which could operate with huge numbers of atoms – up to millions. The most effective quantum methods (for example the Kohn-Sham (KS) method [1]) can work with only hundreds. Therefore, researchers are obliged to use for large nanosystems some less accurate methods with empiric potentials (for example [2,3]).

The Kohn-Sham method is based on density functional theory (DFT) [4]. The orbital-free (OF) approach also follows this theory, however, it operates with the electron density only (without wave functions or orbitals) and if properly developed, can be applied for the simulation of very large systems: up to millions atoms [5]. Several groups [5–13] are working in this area with different success, and the calculation of the kinetic energy is noted as a main problem. In our previous papers [14–16], we suggested that there is no universal way to describe the kinetic energy of different atoms and compounds. We proposed some simple formulas for systems containing atoms of identical types and simulated the dimers and trimers with metallic and covalent bonds. For examples of Al, Si, and C, we obtained equilibrium interatomic distances, binding energies and interbonding angles in good accordance with published data. Now we try to describe how it is possible to extend our approach to systems with different types of atoms.

2. A general description of the OF approach

As it is known, DFT claims that the energy E of the ground state of any quantum system can be found by minimization of the some functional depending only on the electronic density of this system $\rho(\boldsymbol{r})$:

$$E[\rho] = \int \varepsilon(\rho)d\mathbf{r} = \int V(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + \frac{1}{2}\int \varphi(\mathbf{r})\rho(\mathbf{r})d\mathbf{r} + \int \varepsilon_{ex-c}(\rho)d\mathbf{r} + \int \varepsilon_{kin}(\rho)d\mathbf{r}, \tag{1}$$

where $V(\boldsymbol{r})$ is an external potential, $\varphi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'$ is the electrostatic electron potential Hartree, ε_{ex-c} and ε_{kin} are exchange-correlation and kinetic energies (per electron).

Minimization of (1) means solution the following equation:

$$F[p] \equiv \frac{\delta\varepsilon[\rho]}{\delta\rho} = V(\mathbf{r}) + \varphi(\mathbf{r}) + \mu_{ex-c}(\rho) + \mu_{kin}(\rho) = 0, \tag{2}$$

where ρ have to satisfy the condition $\int \rho(\mathbf{r})d\mathbf{r} = N$, N is the number of electrons in the system, $\mu_{ex-c}(\rho) = \frac{\delta\varepsilon_{ex-c}(\rho)}{\delta\rho}$, $\mu_{kin}(\rho) = \frac{\delta\varepsilon_{kin}(\rho)}{\delta\rho}$.

There are some realistic approximations for exchange-correlation potential $\mu_{ex-c}(\rho)$ there; the potential Hartree $\varphi(\mathbf{r})$ may be calculated using Fourier transformations or Poisson equations; the external potential $V(\mathbf{r})$ usually consists of atomic potentials or pseudopotentials. The only real problem is the kinetic potential μ_{kin}.

3. Pseudopotential approach

In practice, the DFT calculations are simpler if one uses pseudopotentials instead of full electron potentials. Therefore, let us rewrite the above equations in the pseudopotential approach, and, for simplicity, let us limit ourselves by s- and p-components of pseudopotentials and a diatomic system. Their distribution on more complicated cases is possible without any trouble. Thus, we will present the total density ρ_{12} as a sum of partial densities: $\rho_{12} = \rho_{12-s} + \rho_{12-p} + \dots$

The electron energy of this system $E_{12} = \int \varepsilon_{12}(\rho_{12-s}, \rho_{12-p}) d\mathbf{r}$ must be minimal with the condition $\int \Big(\rho_{12-s} + \rho_{12-p}\Big) d\mathbf{r} = N_{12}$, where ε_{12} is the electron energy per electron for the two-atomic system with the total number of electrons N_{12}. In the other words, we have to find the density ρ_{12} that satisfies the system of two equations:

$$F_{12-s} = 0, \quad F_{12-p} = 0.$$

Here

$$F_{12-s} \equiv \frac{\delta\varepsilon_{12}}{\delta\rho_{12-s}} = V_{1-s}(r) + V_{2-s}(\mathbf{r}) + \varphi_{12}(\mathbf{r}) + \mu_{12}^{ex-c}(\rho_{12}) + \mu_{12-s}^{kin}(\rho_{12-s}), \tag{3a}$$

$$F_{12-p} \equiv \frac{\delta\varepsilon_{12}}{\delta\rho_{12-p}} = V_{1-p}(\mathbf{r}) + V_{2-p}(\mathbf{r}) + \varphi_{12}(r) + \mu_{12}^{ex-c}(\rho_{12}) + \mu_{12-p}^{kin}(\rho_{12-p}), \tag{3b}$$

where $V_{1-s}(\mathbf{r})$, $V_{2-s}(\mathbf{r})$, $V_{1-p}(\mathbf{r})$ and $V_{2-p}(\mathbf{r})$ are s and p components of pseudopotentials of the first and second atoms, $\varphi_{12}(\mathbf{r})$ and $\mu_{12}^{ex-c}(\rho_{12})$ are the electrostatic and exchange-correlation potentials calculated for the total electron density ρ_{12} of a dimer, $\mu_{12-s}^{kin}(\rho_{12-s})$ and $\mu_{12-p}^{kin}(\rho_{12-p})$ are partial kinetic potentials depending on corresponding partial densities ρ_{12-s} and ρ_{12-p}.

Thus we can write equations for finding ρ_{12-s} and ρ_{12-p}:

$$V_{1-s}(\mathbf{r}) + V_{2-s}(\mathbf{r}) + \varphi_{12}(\mathbf{r}) + \mu_{12}^{ex-c}(\rho_{12}) + \mu_{12-s}^{kin}(\rho_s) = 0, \tag{4a}$$

$$V_{1-p}(\mathbf{r}) + V_{2-p}(\mathbf{r}) + \varphi_{12}(\mathbf{r}) + \mu_{12}^{ex-c}(\rho_{12}) + \mu_{12-p}^{kin}(\rho_p) = 0, \tag{4b}$$

Obviously, for two isolated atoms we can write equations similar to (4a) and (4b):

$$V_{1-s}(\mathbf{r}) + \varphi_1^0(\mathbf{r}) + \mu_1^{ex-c}(\rho_1^0) + \mu_{1-s}^{kin}(\rho_{1-s}^0) = 0, \quad V_{1-p}(\mathbf{r}) + \varphi_1^0(\mathbf{r}) + \mu_1^{ex-c}(\rho_1^0) + \mu_{1-p}^{kin}(\rho_{1-p}^0) = 0 \tag{5a}$$

$$V_{2-s}(\mathbf{r}) + \varphi_2^0(\mathbf{r}) + \mu_2^{ex-c}(\rho_2^0) + \mu_{2-s}^{kin}(\rho_{2-s}^0) = 0, \quad V_{2-p}(\mathbf{r}) + \varphi_2^0(\mathbf{r}) + \mu_2^{ex-c}(\rho_2^0) + \mu_{2-p}^{kin}(\rho_{2-p}^0) = 0 \tag{5b}$$

As ρ_{1-s}^0, ρ_{1-P}^0, ρ_{2-s}^0, and ρ_{2-P}^0 are equilibrium atomic densities taken from DFT calculations, we can write for $V_{1-s}(\mathbf{r})$, $V_{1-p}(\mathbf{r})$, $V_{2-s}(\mathbf{r})$ and $V_{2-p}(\mathbf{r})$:

$$V_{1-s}(\mathbf{r}) = -\varphi_1^0(\mathbf{r}) - \mu_1^{ex-c}(\rho_1^0) - \mu_{1-s}^{kin}(\rho_{1-s}^0), \quad V_{1-p}(\mathbf{r}) = -\varphi_1^0(\mathbf{r}) - \mu_1^{ex-c}(\rho_1^0) - \mu_{1-p}^{kin}(\rho_{1-p}^0), \tag{6a}$$

$$V_{2-s}(\mathbf{r}) = -\varphi_2^0(\mathbf{r}) - \mu_2^{ex-c}(\rho_2^0) - \mu_{2-s}^{kin}(\rho_{2-s}^0), \quad V_{2-p}(\mathbf{r}) = -\varphi_2^0(\mathbf{r}) - \mu_2^{ex-c}(\rho_2^0) - \mu_{2-p}^{kin}(\rho_{2-p}^0). \tag{6b}$$

Putting (6a) and (6b) in (4) we obtain:

$$\varphi_{12}(\mathbf{r}) - \varphi_1^a(\mathbf{r}) - \varphi_2^a(\mathbf{r}) + \mu_{12}^{ex-c}(\rho_{12}) - \mu_1^{ex-c}(\rho_1^0) - \mu_2^{ex-c}(\rho_2^0) + \mu_{12-s}^{kin}(\rho_{12-s}) - \mu_{1-s}^{kin}(\rho_{1-s}^0) - \mu_{2-s}^{kin}(\rho_{2-s}^0) = 0, \tag{7a}$$

$$\varphi_{12}(\mathbf{r}) - \varphi_1^a(\mathbf{r}) - \varphi_2^a(\mathbf{r}) + \mu_{12}^{ex-c}(\rho_{12}) - \mu_1^{ex-c}(\rho_1^0) - \mu_2^{ex-c}(\rho_2^0) + \mu_{12-p}^{kin}(\rho_{12-p}) - \mu_{1-p}^{kin}(\rho_{1-p}^0) - \mu_{2-p}^{kin}(\rho_{2-p}^0) = 0. \tag{7b}$$

The kinetic dimer functionals $\mu_{12-s}^{kin}(\rho_{12-s})$ and $\mu_{12-p}^{kin}(\rho_{12-p})$ may be presented as follows:

$$\mu_{12-s}^{kin}(\rho_{12-s}) = \mu_{1-s}^{kin}(\rho_{1-s}^0) + \mu_{2-s}^{kin}(\rho_{2-s}^0) + \Delta\mu_{12-s}^{kin}(\rho_{12-s}), \tag{8a}$$

$$\mu_{12-p}^{kin}(\rho_{12-p}) = \mu_{1-p}^{kin}(\rho_{1-p}^0) + \mu_{2-p}^{kin}(\rho_{2-p}^0) + \Delta\mu_{12-p}^{kin}(\rho_{12-p}), \tag{8b}$$

where $\Delta\mu_{12-s}^{kin}(\rho_{12-s})$ and $\Delta\mu_{12-p}^{kin}(\rho_{12-p})$ are unknown functions of partial densities of the two-atomic system. These functions must approach zero if the interatomic distance approaches to infinity. Thus we can take the following simple approximation for them:

$$\Delta\mu_{12-s}^{kin}(\rho^{)}_{12-s} \approx \nu_{A-s}^{kin}(\rho^{)}_{12-s} - \nu_{A-s}^{kin}(\rho_{1-s}^0) - \nu_{A-s}^{kin}(\rho_{2-s}^0), \tag{9a}$$

$$\Delta\mu_{12-p}^{kin}(\rho^{)}_{12-p} \approx \nu_{A-p}^{kin}(\rho^{)}_{12-p} - \nu_{A-p}^{kin}(\rho_{1-p}^0) - \nu_{A-p}^{kin}(\rho_{2-p}^0), \tag{9b}$$

where $\nu_{A-s}^{kin}(\rho_s)$ and $\nu_{A-p}^{kin}(\rho_p)$ are some functions having the same kind for single atoms and for dimers formed from atoms of the same type A.

We can solve these equations with some fitting functions ν_{A-s}^{kin} and ν_{A-p}^{kin} and then calculate the total energy. We find the test functions from the simple request: they must lead to the equilibrium interatomic distances and binding energy for dimers. We hope that these functions will be suitable for more complicated systems in future.

The electron energy of a dimer E^{el}_{dim} contains the electrostatic energy:

$$E^{e-stat}_{12} = \int [V_{1-s}(\mathbf{r}) + V_{2-s}(\mathbf{r})]\,\rho_{12-s}d\mathbf{r} + \int [V_{1-p}(\mathbf{r}) + V_{2-p}(\mathbf{r})]\,\rho_{12-p}d\mathbf{r} + \frac{1}{2}\int \varphi_{12}(\mathbf{r})\rho_{12}d\mathbf{r}, \tag{10}$$

the exchange-correlation energy $E^{ex-c}_{12} = \int \varepsilon^{ex-c}_{12}(\rho_{12})d\mathbf{r}$ and the kinetic energy:

$$E^{kin}_{12} = E^{kin}_{1} + E^{kin}_{2} + \iint \left[\nu^{kin}_{12-s}(\rho_{12-s})d\rho_{12-s} + \nu^{kin}_{12-s}(\rho_{12-p})d\rho_{12-s}\right]d\mathbf{r}. \tag{11}$$

To find the equilibrium distance and the total energy E^{tot}_{dim}, we need to add the repelling energy $E^{rep}_{12} = \dfrac{Z_1 Z_2}{|\mathbf{R}_1 - \mathbf{R}_2|}$, where Z_1 and Z_2 are positive charges of atomic ions with coordinates $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$. Thus $E^{tot}_{\text{dim}} = E^{e-stat}_{12} + E^{ex-c}_{12} + E^{kin}_{12} + E^{rep}_{12}$. The binding energy for a dimer (per one atom) would be calculated as follows: $E_b = \frac{1}{2}\left(E^{tot}_{\text{dim}} - 2E_a\right)$, where E_a is the atomic energy.

4. Dimers with identical atoms

We took Al, Si, and C as test elements. We used the FHI98pp [17] package as a generator of pseudo-potentials and equilibrium partial electron densities. We calculated exchange and correlation potentials in the local density approach [18,19]. Studied atoms were located in a cubic cell of the L size (L=30 a.u.; 1 a.u. = 0.529 Å). The cell was divided on $150 \times 150 \times 150$ elementary sub-cells for the integration with the step ΔL of 0.2 a.u. The results of these calculations were compared with published data.

We used the same types of kinetic functions μ^{kin}_s and μ^{kin}_p for isolated atoms and dimers and trimers, however they were found different for different types of atoms. Namely, we used
for Al: $\nu^{kin}_s = 1.0\rho_s^{1/4.5}$; $\nu^{kin}_p = 22.0\rho_p^{1/1.5}$;
for Si: $\nu^{kin}_s = 8.0\rho_s^{1/1.5}$; $\nu^{kin}_p = 1.6\rho_p^{1/3}$;
for C: $\nu^{kin}_s = 1.75\rho_s^{1/3}$; $\nu^{kin}_p = 1.8\rho_p^{1/3}$.

Calculated values of interatomic distances and binding energies for the Al_2, Si_2, and C_2 dimers are collected in Table 1 in comparison with other data. Agreement is rather satisfactory, when one considers that other calculated data are often differing from experimental results and each other.

TABLE 1. Equilibrium distances d and binding energies E_b (absolute values, per atom) for Si_2, Al_2 and C_2 in comparison with known data

Dimer	Source	d, Å	E_b,eV
Si_2	Our OF method	2.2	1.8
	Other calculations	2.21^a 2.23^b	1.599^a 1.97^b
	Experiment	2.24^c	3.0^c
Al_2	Our OF method	2.8	1.4
	Other calculations	2.95^d 2.51^e	1.23^d 1.55^e
	Experiment	2.56^f	1.56^f
C_2	Our OF method	1.4	3.0
	Other calculations	1.24^g 1.36^h	2.6^g 2.7^h
	Experiment	1.24^i	3.1^i

Notations: [a][20], [b][21], [c][22], [d][23],[e][24], [f][25], [g][26], [h][27], [i][28].

5. Dimers with different atoms

Let us rewrite equations (8a) and (8b) for a dimer contained atoms of types A and B:

$$\mu^{kin}_{AB-s}(\rho_{AB-s}) = \mu^{kin}_{A-s}(\rho^0_{A-s}) + \mu^{kin}_{B-s}(\rho^0_{B-s}) + \Delta\mu^{kin}_{AB-s}(\rho_{AB-s}), \tag{12a}$$

$$\mu^{kin}_{AB-p}(\rho_{AB-p}) = \mu^{kin}_{A-p}(\rho^0_{A-p}) + \mu^{kin}_{B-p}(\rho^0_{B-p}) + \Delta\mu^{kin}_{AB-p}(\rho_{AB-p}). \tag{12b}$$

The functions $\Delta\mu^{kin}_{AB-s}(\rho_{AB-s})$ and $\Delta\mu^{kin}_{AB-p}(\rho_{AB-p})$ have to be approximately equal to atomic functions $\Delta\mu^{kin}_{A-s(p)}$ or $\Delta\mu^{kin}_{B-s(p)}$ near atoms A or B, but they have to be mixtures of the atomic functions in the whole space. It seems to us that the simplest way to construct the functions $\Delta\mu^{kin}_{AB-s(p)}$ and $\mu^{kin}_{AB-s(p)}$ is to summarize the atomic functions with some weights:

$$\Delta\mu^{kin}_{AB-s}(\rho_{AB-s}) = W_{A-s}\Delta\mu^{kin}_{A-s}(\rho_{AB-s}) + W_{B-s}\Delta\mu^{kin}_{B-s}(\rho_{AB-s}); \tag{13a}$$

$$\Delta\mu^{kin}_{AB-p}(\rho_{AB-p}) = W_{A-p}\Delta\mu^{kin}_{A-p}(\rho_{AB-p}) + W_{B-p}\Delta\mu^{kin}_{B-p}(\rho_{AB-p}). \tag{13b}$$

For $\Delta\mu^{kin}_{A-s(p)}$ and $\Delta\mu^{kin}_{B-s(p)}$ we propose the following approximations:

$$\Delta\mu^{kin}_{A-s}(\rho_{AB-s}) \approx \nu^{kin}_{A-s}(\rho_{AB-s}) - \nu^{kin}_{A-s}(\rho^0_{A-s}) - \nu^{kin}_{A-s}(\rho^0_{B-s}), \tag{14a}$$

$$\Delta\mu^{kin}_{B-s}(\rho_{AB-s}) \approx \nu^{kin}_{B-s}(\rho_{AB-s}) - \nu^{kin}_{B-s}(\rho^0_{A-s}) - \nu^{kin}_{B-s}(\rho^0_{B-s}), \tag{14b}$$

$$\Delta\mu^{kin}_{A-p}(\rho_{AB-p}) \approx \nu^{kin}_{A-p}(\rho_{AB-p}) - \nu^{kin}_{A-p}(\rho^0_{A-p}) - \nu^{kin}_{A-p}(\rho^0_{B-p}), \tag{14c}$$

$$\Delta\mu^{kin}_{B-p}(\rho_{AB-p}) \approx \nu^{kin}_{B-p}(\rho_{AB-p}) - \nu^{kin}_{B-p}(\rho^0_{A-p}) - \nu^{kin}_{B-p}(\rho^0_{B-p}), \tag{14d}$$

where ν^{kin}_{A-s}, ν^{kin}_{A-p}, ν^{kin}_{B-s} and ν^{kin}_{B-p} are functions related to atoms A and B. For Al, Si and C they are found in the previous Section.

The weights W_{A-s}, W_{A-p}, W_{B-s} and W_{B-P} may be determined through Gauss functions fitted to atomic densities:

$$W_{A-s} = \frac{\alpha_{A-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-s}}\right)}{\alpha_{A-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-s}}\right) + \alpha_{B-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-s}}\right)}; \tag{15a}$$

$$W_{B-s} = \frac{\alpha_{B-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-s}}\right)}{\alpha_{A-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-s}}\right) + \alpha_{B-s}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-s}}\right)}; \tag{15b}$$

$$W_{A-p} = \frac{\alpha_{A-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-p}}\right)}{\alpha_{A-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-p}}\right) + \alpha_{B-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-p}}\right)}; \tag{15c}$$

$$W_{B-p} = \frac{\alpha_{B-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-p}}\right)}{\alpha_{A-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_A)^2}{\beta_{A-p}}\right) + \alpha_{B-p}\exp\left(-\frac{(\mathbf{r}-\mathbf{R}_B)^2}{\beta_{B-p}}\right)}. \tag{15d}$$

An example of fitting of the densities and weights is demonstrated in Figure 1. Values for α and β for Si, Al, C and O are presented in Table 2.

TABLE 2. Parameters of weight functions (α and β) for Si, Al, C and O atoms

Type of atom	α_s	α_p	β_s	β_p
Si	0.065	0.040	3.5	4.5
Al	0.065	0.005	3.5	4.5
C	0.200	0.160	1.5	1.8
O	0.300	0.450	1.0	1.5

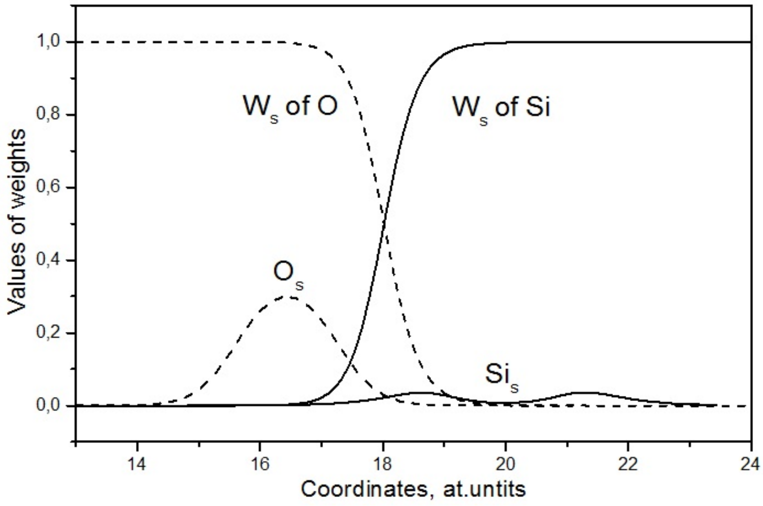

FIG. 1. The s-densities and the weights W$_s$ for oxygen (dashed) and silicon atoms (solid)

We fulfilled calculations for the SiC, SiAl, AlC, SiO, CO, and AlO dimers with parameters shown in Table 2. The kinetic functions for oxygen $\nu_s^{kin} = 1.7\rho_s^{1/3} - 1.0\rho_s$ and $\nu_p^{kin} = 1.5\rho_p^{1/3.5} - 1.0\rho_p$ have been found through simulation of the SiO dimer and then they were used for other oxygen contained dimers. Results of calculations are presented in Table 3. Unfortunately, we did not find published data for the all studied heteroatomic dimers. Therefore, we compared our OF results also with results calculated by us in the framework of the KS DFT approach using the well-known package FHI96md [17].

TABLE 3. Equilibrium distances d and energies of dissociation E_d (absolute values) for SiC, SiAl, AlC, SiO, CO, and AlO

Dimer	Source	d, Å	E_d,eV
SiC	Our OF calculations	1.9	6.9
	Published calculations	1.8[a]	7.7[a]
	Our KS FHI96md calculations	1.69	6.66
SiAl	Our OF calculations	2.5	3.8
	Our KS FHI96md calculations	2.30	3.10
AlC	Our OF calculations	2.0	6.1
	Our KS FHI96md calculations	1.83	4.32
SiO	Our OF calculations	1.6	7.0
	Our KS FHI96md calculations	1.51	12.06
	Experiment	1.52[b]	7.2[b]
CO	Our OF calculations	1.0	9.5
	Our KS FHI96md calculations	1.11	15.96
	Experiment	1.13[c]	9.6[c]
AlO	Our OF calculations	1.8	3.0
	Our KS FHI96md calculations	1.55	9.0
	Experiment	1.62[c]	5.27[c]

Notations: [a][30], [b][31], [c][32].

One can see from Table 3 that our OF equilibrium distances slightly exceed the experimental ones as well as the KS calculation results, except the CO dimer. As for the dissociation energy, the OF results for the SiO and CO dimers are closer to experimental data than the KS ones. The OF result for SiC correlates with our KS and known calculated values (there is no experimental data). OF calculated energies for the Al contained dimers are rather far from experimental values and from results of KS calculations. The reason for this discrepancy requires future investigation; however, it is remarkable that the KS results are also far from experimental energies in many cases. As a whole, we can conclude that the OF method is able to give us a rather satisfactory information on interatomic distances and energies of systems containing different atoms.

6. Conclusion

We showed the possibility for simulating the interactions of atoms of non-identical types in the framework of the orbital-free version of the density functional theory. For this purpose, we used a rather simple technique, namely: first, the atomic kinetic functions were found for homo-atomic dimers Si_2, Al_2, C_2 and for the SiO dimer; second, some atomic weights were proposed using Gaussians associated with atomic densities; third, kinetic functions for hetero-atomic dimers were constructed. Equilibrium interatomic distances and dissociation energies for the SiC, SiAl, AlC, SiO and CO dimers were found to be in satisfactory agreement with the Kohn-Shem calculations and experimental data.

As the calculation of the kinetic energy is a key point in the modeling of polyatomic systems in the orbital-free approach, it is possible to consider that our work opens a direct way to design an effective modeling method for complicated nanosystems and macromolecules with a large number of atoms.

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