In this work, we have used the exchange-only optimized effective potential in the self-consistent calculations of the density functional Kohn-Sham equations for simple metal clusters in stabilized jellium model with self-compression. The results for the closed-shell clusters of Al, Li, Na, K, and Cs with \( N = 2, 8, 18, 20, 34, \) and 40 show that the clusters are 3% more compressed here than in the local spin density approximation. On the other hand, in the LSDA, neglecting the correlation results in a contraction by 1.4%.

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I. INTRODUCTION

The Kohn-Sham (KS) \[1\] density functional theory (DFT) \[2\] is one of the most powerful techniques in electronic structure calculations. However, the exact form of the exchange-correlation functional is still unknown and, in practice, one must use approximations. The accuracy of the predictions of the properties depends on how one approximates this functional. The simplest one is the local spin density approximation (LSDA) in which one uses the properties of the uniform electron gas locally \[1\]. This approximation is in principle appropriate for systems in which the variations of the spin densities \( n_s \) are sufficiently slow. For finite systems and surfaces which are highly inhomogeneous, the generalized gradient approximation (GGA) \[3\] is more appropriate. In spite of the success of the LSDA and GGA, it is observed that in some cases these approximations fail to predict even qualitatively correct behaviors \[4, 5, 6, 7\]. On the other hand, appropriate self-interaction corrected versions of these approximations are observed to lead to correct behaviors \[8, 9\]. These observations motivates one to use functionals in which the self-interaction contribution is removed exactly. One of the functionals, which satisfies this constraint, is the exact exchange (EEX) orbital dependent functional. Using the EEX functional leads to the correct asymptotic behavior of the KS potential as well as to correct results for the high density limit in which the exchange energy is dominated \[10\]. Although neglecting the correlation effects in orbital dependent functionals fails to reproduce the dispersion forces such as the van der Waals forces \[10, 11\], the EEX in some respects is advantageous over the local and semi-local approximations \[11, 12\]. To obtain the local exchange potential from the orbital dependent functional, one should solve the optimized effective potential (OEP) integral equation. Recently, K"ummel and Perdew \[13, 14\] have invented an iterative method which allows one to solve the OEP integral equation accurately and efficiently even for three dimensional systems. This method is used in this work.

To simplify the cluster problem, one notes that the properties of alkali metals are dominantly determined by the delocalized valence electrons. In these metals, the Fermi wavelengths of the valence electrons are much larger than the metal lattice constants and the pseudo-potentials of the ions do not significantly affect the electronic structure. This fact allows one to replace the discrete ionic structure by a homogeneous positive charge background which is called jellium model (JM). In its simplest form, one applies the JM to metal clusters by replacing the ions of an \( N \)-atom cluster with a sphere of uniform positive charge density and radius \( R = (zN)^{1/3}r_s \), where \( z \) is the valence of the atom and \( r_s \) is the bulk value of the Wigner-Seitz (WS) radius for valence electrons \[13, 16, 17\]. Assuming the spherical geometry is justified only for closed-shell clusters which is the subject in this work. However, it is a known fact that the JM has some drawbacks \[13, 19\]. The stabilized jellium model (SJM) in its original form \[20\] was the first attempt to overcome the deficiencies of the JM and still keeping the simplicity of the JM. Application of the SJM to simple metals and metal clusters has shown significant improvements over the JM results \[20\]. However, for small metal clusters the surface effects are important and the cluster is self-compressed due to its surface tension. This effect has been successfully taken into account by the SJM which is called SJM with self-compression (SJM-SC) \[21, 22\]. Application of the LSDA-SJM-SC to neutral metal clusters has shown that the equilibrium \( r_s \) values of small clusters are smaller than their bulk counterparts and approaches to it for very large clusters. This trend is consistent with the results of \emph{ab. initio} calculations \[23, 24\].

In this work we have used the EEX-SJM-SC to obtain the equilibrium sizes and energies of closed-shell neutral \( N \)-electron clusters of Al, Li, Na, K, and Cs for \( N = 2, 8, 18, 20, 34, \) and 40 (for Al, \( N = 18 \) corresponds to \( Al_{18} \) cluster and other values do not correspond to a real \( Al_{n} \)). In order to have an estimate for the self-interaction effects, we have repeated the calculations for exchange-only local spin density approximation (x-LSDA) in which the spin-polarized version of the
Dirac form, \( E_x = c_x \int dr \, n^{4/3} \), is used. Comparison of the results shows that (except for \( N = 40 \) in Al case) the relation \( \bar{E}_{EEX} < \bar{E}_{x-LSDA} < \bar{E}_{LSDA} \). The organization of this paper is as follows. In section II we explain the calculational schemes. Section III is devoted to the results of our calculations and finally, we conclude this work in section IV.

II. CALCULATIONAL SCHEMES

In this section we first explain how to implement the exact exchange in the SJM, and then will explain the procedure for the OEP calculations.

A. Exact exchange stabilized jellium model

As in the original SJM\[^{20}\], here the Ashcroft empty core pseudo-potential\[^{25}\] is used for the interaction of an ion of charge \( z \) with an electron at a relative distance \( r \):

\[
w(r) = \begin{cases} -2z/r, & (r > r_c) \\ 0, & (r < r_c) \end{cases}
\]

The core radius, \( r_c \), will be fixed by setting the pressure of the bulk system equal to zero. In the EEX-SJM, the average energy per valence electron in the bulk with density \( n \) is given by

\[
\varepsilon(n) = t_s(n) + \varepsilon_x(n) + \bar{\omega}_R(n, r_c) + \varepsilon_M(n),
\]

with

\[
t_s(n) = c_k n^{2/3},
\]

\[
\varepsilon_x(n) = c_x n^{1/3},
\]

\[
c_k = \frac{3}{5} (3\pi^2)^{2/3}, \quad c_x = \frac{3}{2} (3/\pi)^{1/3}.
\]

All equations throughout this paper are expressed in Rydberg atomic units. Here \( t_s \) and \( \varepsilon_x \) are the kinetic and exchange energy per particle, respectively. \( \bar{\omega}_R \) is the average value of the repulsive part of the pseudo-potential (\( \bar{\omega}_R = 4\pi n^2 r_c^2 \)), and \( \varepsilon_M \) is the average Madelung energy. Demanding zero pressure for the bulk system at equilibrium yields:

\[
\{ 2t_s(n) + \varepsilon_x(n) + 12\pi n r_c^2 + \varepsilon_M(n) \} \big|_{n=n^B} = 0.
\]

Solution of this equation for \( r_c \) gives

\[
r_c(r_s^B) = \frac{(r_s^B)^{3/2}}{3} \left\{ -2t_s(r_s) - \varepsilon_x(r_s) - \varepsilon_M(r_s) \right\}^{1/2}_{r_s=r_s^B}.
\]

In Fig. 1 we have plotted the core radii for different values of \( r_s^B \) which assume 2.07, 3.28, 3.99, 4.96, and 5.63 for Al, Li, Na, K, and Cs, respectively. The result is compared with the case in which the correlation energy is also incorporated (see Eq.(26) of Ref.\[^{20}\]). As is seen, to stabilize the bulk system in the EEX case, the core radii assume smaller values.

As in the original SJM\[^{20}\] (but in the absence of the correlation energy component), at equilibrium density we have

\[
\langle \delta v \rangle_{WS} = -\frac{1}{3} [2t_s(n^B) + \varepsilon_x(n^B)].
\]

Here, \( \langle \delta v \rangle_{WS} \) is the average of the difference potential over the WS cell and the difference potential, \( \delta v \), is defined as the difference between the pseudo-potential of a lattice of ions and the electrostatic potential of the jellium positive background. Once the values of \( \langle \delta v \rangle_{WS} \) and \( r_c \) as functions of \( r_s^B \) are found, the EEX-SJM total energy of a cluster becomes

\[
E_{EEX-SJM}[n_\uparrow, n_\downarrow, r_s, r_s^B] = E_{EEX-JM}[n_\uparrow, n_\downarrow, r_s] + (\varepsilon_M + \bar{\omega}_R) \int dr \, n_+ (r)
\]

\[
+ \langle \delta v \rangle_{WS} \int dr \, \Theta(r) [n(r) - n_+ (r)].
\]

Here,

\[
E_{EEX-JM}[n_\uparrow, n_\downarrow, r_s] = T_s[n_\uparrow, n_\downarrow] + E_x[n_\uparrow, n_\downarrow] + \frac{1}{2} \int dr \, \phi([n_\uparrow, n_\downarrow]; r) [n(r) - n_+ (r)],
\]

\[
E_x = \sum_{\sigma=\uparrow,\downarrow} \sum_{i,j=1}^{N_x} \int dr \, dr' \frac{\phi^*_{i\sigma}(r) \phi^*_{j\sigma}(r') \phi_{i\sigma}(r) \phi_{j\sigma}(r')}{|r - r'|},
\]

FIG. 1: Pseudo-potential core radii in atomic units for different \( r_s^B \) values.
\[ \phi([n, n_+]; \mathbf{r}) = 2 \int d\mathbf{r}' \frac{n(\mathbf{r}') - n_+(\mathbf{r}')} {|| \mathbf{r} - \mathbf{r}' ||}, \]

\[ n(\mathbf{r}) = \sum_{\sigma = \uparrow, \downarrow} \sum_{i=1}^{N_\sigma} | \phi_{i\sigma}(\mathbf{r}) |^2, \]

\[ n_+(\mathbf{r}) = n_0(R - r); \quad n = \frac{3}{4\pi r_s^3}. \]

To obtain the equilibrium size and energy of an \( N \)-atom cluster in EEX-SJM-SC, we solve the equation

\[ \frac{\partial}{\partial r_s} E(N, r_s, \rho_c) \bigg|_{r_s = \bar{r}_s(N)} = 0, \]

where \( N \) and \( \rho_c \) are kept constant and \( E \) is given by Eq. (9). The procedure for the x-LSDA is the same as above except for that the Dirac exchange energy must be used.

### B. The OEP equations

Kümmel and Perdew\(^\text{14}\) have proved, in a simple way, that the OEP integral equation is equivalent to

\[ \sum_{i=1}^{N_\sigma} \psi^*_i(\mathbf{r}) \phi_{i\sigma}(\mathbf{r}) + c.c. = 0. \]

\( \phi_{i\sigma} \) are the self-consistent KS orbitals and \( \psi_{i\sigma} \) are orbital shifts. The self-consistent orbital shifts and the local exchange potentials are obtained from the iterative solutions of inhomogeneous KS equations. Taking spherical geometry for the jellium background and inserting

\[ \phi_{i\sigma}(\mathbf{r}) = \frac{\chi_{i\sigma}(r)}{r} Y_{l_i, m_i}(\Omega), \]

and

\[ \psi_{i\sigma}(\mathbf{r}) = \frac{\xi_{i\sigma}(r)}{r} Y_{l_i, m_i}(\Omega), \]

in to the inhomogeneous KS equation (Eq.(21) of Ref.\(^\text{14}\)) one obtains\(^\text{22}\)

\[ \left[ \frac{d^2}{dr^2} + \varepsilon_{i\sigma} - v_{\text{eff}}(r) - l_i(l_i + 1) r^2 \right] \xi_{i\sigma}(r) = q_{i\sigma}(r). \]

The right hand side of Eq. (19) can be written as

\[ q_{i\sigma}(r) = q_{i\sigma}^{(1)}(r) + q_{i\sigma}^{(2)}(r), \]

with

\[ q_{i\sigma}^{(1)}(r) = [v_{xc\sigma}(r) - \bar{v}_{xc\sigma} + \bar{u}_{xc\sigma}] \chi_{i\sigma}(r), \]

and

\[ q_{i\sigma}^{(2)}(r) = 2 \sum_{j=1}^{N_\sigma} \sum_{l=l_i-l_j}^{l_i+l_j} \frac{4\pi}{2l+1} \chi_{j\sigma}(r) B_{\sigma}(i, j, l; r) \times [I(l_j m_j, l_i m_i, l m_j - m_i)]^2. \]

The quantities \( B \) and \( I \) in Eq. (24) are defined as

\[ B_{\sigma}(i, j, l; r) = \int_{r'=0}^{r} dr' \chi_{i\sigma}(r') \chi_{j\sigma}(r') r'^l \]

\[ + \int_{r'=r}^{\infty} dr' \chi_{i\sigma}(r') \chi_{j\sigma}(r') r'^l \]

\[ I(l_j m_j, l_i m_i, l m_j - m_i) = \int d\Omega \ Y_{l_j m_j}(\Omega) Y_{l_i m_i}(\Omega) Y_{l m_j}(\Omega), \]

and the bar over \( \bar{u} \) implies average over \( m_i \) and \( m_j \). Also, the expression for \( \bar{u}_{xc\sigma} \) reduces to

\[ \bar{u}_{xc\sigma} = -2 \sum_{j=1}^{N_\sigma} \sum_{l=l_i-l_j}^{l_i+l_j} \frac{4\pi}{2l+1} [I(l_j m_j, l_i m_i, l m_j - m_i)]^2 \]

\[ \times \int_{0}^{\infty} dr \chi_{i\sigma}(r) \chi_{j\sigma}(r) B_{\sigma}(i, j, l; r). \]

The procedure for the self-consistent iterative solutions of the OEP equations is explained in Refs.\(^\text{14,26}\).

In Fig. 2 the self-consistent source terms \( q_{i\sigma}(r) \) of Eq. (19) are plotted for the equilibrium size of Na\(_{18}\) cluster. The corresponding orbital shifts \( \xi_{i\sigma}(r) \) are shown in Fig. 4.

### III. RESULTS AND DISCUSSION

We have used the EEX-SJM-SC to obtain the equilibrium sizes and energies of closed-shell 2, 8, 18, 20, 34, and 40-electron neutral clusters of Al, Li, Na, K, and Cs. In Table I we have listed the equilibrium \( r_s \) values, total energies and exchange energies. As is seen, the equilibrium \( r_s \) values of the clusters are almost the same up to 3 decimals for the KLI and OEP schemes whereas, there are significant differences between the OEP, x-LSDA, and LSDA values. As an example, we have plotted the equilibrium \( r_s \) values of the closed-shell K\(_N\) clusters in Fig. 4. It shows that the LSDA predicts larger cluster sizes than the x-LSDA and OEP.
To illustrate the trend in the $\bar{r}_s$ values, we plot the difference $(\bar{r}_s^{\text{LSD}} - \bar{r}_s^{\text{KLI}})$ for all species in Fig. 5. One notes that for a given element, the difference is larger for smaller clusters. On the other hand, the difference for the lower-density element is higher. However, the difference is about 3% on average. We therefore conclude that the EEX-SJM-SC predicts smaller bond lengths compared to the LSDA-SJM-SC. Comparison of the $\bar{r}_s$ values for the LSDA and x-LSDA shows that bond lengths in the LSDA is about 1.4% larger on average. This difference should be attributed to the correlation effects. On the other hand, the same comparison between x-LSDA and KLI shows that, except for $N = 40$ in Al, $\bar{r}_s^{\text{x-LSDA}} > \bar{r}_s^{\text{KLI}}$ by 1.5% on average. This difference is due to the self-interaction effects in the Dirac form for the exchange functional.

Comparison of the equilibrium total energies of the OEP and KLI shows that OEP energies are on average 0.02% more negative. This result should be compared to the simple JM results, which is 1.2%. On the other hand, comparison of the exchange energies shows that on the average, the exchange energies in OEP is 0.34% more negative than those in the KLI.

In Table II, we have listed the lowest and highest occupied KS eigenvalues for different schemes. As in the simple JM, the OEP KS eigenvalue bands are contracted relative to those of the KLI. That is, for all $N$, the relation $\Delta_{\text{OEP}} < \Delta_{\text{KLI}}$ holds. Here, $\Delta = \varepsilon_H - \varepsilon_L$ is the difference between the maximum occupied and minimum
occupied KS eigenvalues. For the same external potential, the OEP and KLI results coincide for two-electron systems and $\Delta = 0$. The results in Table I show that the maximum relative contraction, $|\Delta_{\text{OEP}}^{\text{OEP}} - \Delta_{\text{KLI}}^{\text{KLI}}|/\Delta_{\text{KLI}}^{\text{KLI}}$, is 2.7% which corresponds to Cs$_{18}$.

The same comparisons between OEP and x-LSDA show that $E_{\text{OEP}}^{\text{OEP}} < E_{\text{x-LSDA}}^{\text{x-LSDA}}$ by 5.2% on average, and $E_{\text{x-LSDA}}^{\text{OEP}} < E_{\text{x-LSDA}}^{\text{x-LSDA}}$ by 11% on average. The band widths do not show any regular pattern, however, in the OEP the bands mostly contract relative to the x-LSDA.

Finally, we compare the results of LSDA and x-LSDA, which will show the correlation effects. As is seen in Table II the total energies are close to each other for the high-density cases. That is, in the high density limit the exchange dominates the correlation. However, the total energies in the LSDA are more negative by 10% on average which is due to the correlation effects. On the other hand, the difference in the exchange energies is on average which is due to the correlation effects. The widths of the occupied bands, mostly contract relative to the x-LSDA. 

The same comparisons between OEP and x-LSDA show a difference in 3% on average. The total energies in the OEP are more negative than the KLI by 0.02% on the average. It should be mentioned that in the simple JM the KLI and OEP total energies for Al were positive (except for $N = 2$). On the other hand, the exchange energies in the OEP is about 0.34% more negative than that in the KLI. Comparison of the OEP and x-LSDA shows a difference of 5.2% in the total energies and 11% in the exchange. The difference in the exchange energies of LSDA and x-LSDA is small (about 0.96%) whereas the total energy in the LSDA is about 10% more negative which is due to the correlation effects. The widths of the occupied bands, $\varepsilon_{\text{H}} - \varepsilon_{\text{L}}$ in the OEP are contracted relative to those in the KLI by at most 2.7%.

IV. SUMMARY AND CONCLUSION

In this work, we have considered the exact-exchange stabilized jellium model with self-compression in which we have used the exact orbital-dependent exchange functional. This model is applied for the simple metal clusters of Al, Li, Na, K, and Cs. For the local exchange potential in the KS equation, we have solved the OEP integral equation by the iterative method. By finding the minimum energy of an $N$-atom cluster as a function of $r_s$, we have obtained the equilibrium sizes and energies of the closed-shell clusters ($N = 2, 8, 18, 20, 34, 40$) for the four schemes of LSDA, KLI, OEP, and x-LSDA. The results show that in the EEX-SJM, the clusters are more contracted relative to the x-LSDA-SJM, i.e., 1.5% more contraction on average. The KLI and OEP results show equal values (up to three decimals) for the equilibrium $r_s$ values. The equilibrium sizes in LSDA and x-LSDA differ by 1.4% on average. In the LSDA and KLI the difference is 3% on average. The total energies in the OEP are more negative than the KLI by 0.02% on the average. It should be mentioned that in the simple JM the KLI and OEP total energies for Al were positive (except for $N = 2$). On the other hand, the exchange energies in the OEP is about 0.34% more negative than that in the KLI. Comparison of the OEP and x-LSDA shows a difference of 5.2% in the total energies and 11% in the exchange. The difference in the exchange energies of LSDA and x-LSDA is small (about 0.96%) whereas the total energy in the LSDA is about 10% more negative which is due to the correlation effects. The widths of the occupied bands, $\varepsilon_{\text{H}} - \varepsilon_{\text{L}}$ in the OEP are contracted relative to those in the KLI by at most 2.7%.

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TABLE I: Equilibrium sizes, $\bar{r}_s$, in bohrs, the absolute values of total and exchange energies in rydbergs are compared for KLI, OEP, x-LSDA, and LSDA schemes. In the LSDA, the total energies include the correlation energies as well.

| Atom | $r^b$ | $N$ | $\bar{r}_s$ | $-\bar{E}$ | $\bar{r}_s$ | $-\bar{E}$ | $\bar{r}_s$ | $-\bar{E}$ | $\bar{r}_s$ | $-\bar{E}$ |
|------|-------|-----|-------------|----------|-------------|----------|-------------|----------|-------------|----------|
| Al** | 2.07  | 2   | 1.430       | 1.5700   | 0.9253      | 1.430    | 1.5700      | 0.9253   | 1.430       | 1.5700   |
|      |       | 8   | 1.744       | 5.8640   | 3.0018      | 1.744    | 5.8647      | 3.0699   | 1.775       | 5.5768   |
|      |       | 18  | 1.876       | 12.7709  | 7.9467      | 1.876    | 12.7734     | 7.9760   | 1.898       | 12.3315  |
|      |       | 20  | 1.846       | 14.3309  | 8.8532      | 1.847    | 14.3311     | 8.8706   | 1.869       | 13.8729  |
|      |       | 34  | 1.928       | 23.9914  | 14.9571     | 1.928    | 23.9968     | 15.0339  | 1.944       | 23.3442  |
|      |       | 40  | 1.901       | 28.2841  | 17.5064     | 1.901    | 28.2863     | 17.5348  | 1.913       | 27.6468  |
| Li   | 3.28  | 2   | 2.698       | 1.0076   | 0.5748      | 2.698    | 1.0076      | 0.5748   | 2.756       | 0.9247   |
|      |       | 8   | 2.966       | 3.9138   | 2.5011      | 2.966    | 3.9144      | 2.5357   | 3.013       | 3.7326   |
|      |       | 18  | 3.080       | 8.6776   | 5.0261      | 3.080    | 8.6798      | 5.0506   | 3.117       | 8.3934   |
|      |       | 20  | 3.059       | 9.6670   | 5.5148      | 3.059    | 9.6682      | 5.5553   | 3.094       | 9.3791   |
|      |       | 34  | 3.134       | 16.3774  | 9.4868      | 3.134    | 16.3823     | 9.5289   | 3.157       | 15.9553  |
|      |       | 40  | 3.111       | 19.1876  | 10.9835     | 3.111    | 19.1898     | 11.0652  | 3.136       | 18.7942  |
| Na   | 3.99  | 2   | 3.403       | 0.8409   | 0.4785      | 3.403    | 0.8409      | 0.4785   | 3.475       | 0.7721   |
|      |       | 8   | 3.664       | 3.2841   | 1.8579      | 3.664    | 3.2864      | 1.8632   | 3.719       | 3.1343   |
|      |       | 18  | 3.784       | 7.3064   | 4.1549      | 3.784    | 7.3084      | 4.1772   | 3.821       | 7.0700   |
|      |       | 20  | 3.758       | 8.1240   | 5.0669      | 3.758    | 8.1251      | 5.0794   | 3.800       | 7.8873   |
|      |       | 34  | 3.834       | 13.7980  | 7.8340      | 3.834    | 13.8028     | 7.8751   | 3.862       | 13.4458  |
|      |       | 40  | 3.813       | 16.1410  | 9.0432      | 3.813    | 16.1431     | 9.0632   | 3.843       | 15.8198  |
| K    | 4.96  | 2   | 4.354       | 0.6882   | 0.3920      | 4.354    | 0.6882      | 0.3920   | 4.443       | 0.6321   |
|      |       | 8   | 4.609       | 2.6951   | 1.5054      | 4.609    | 2.6955      | 1.5098   | 4.680       | 2.5738   |
|      |       | 18  | 4.734       | 6.0102   | 3.6359      | 4.734    | 6.0121      | 3.8360   | 4.781       | 5.8178   |
|      |       | 20  | 4.710       | 6.6722   | 3.6887      | 4.710    | 6.6753      | 3.7002   | 4.760       | 6.4820   |
|      |       | 34  | 4.787       | 11.3534  | 6.3392      | 4.787    | 11.3579     | 6.3785   | 4.824       | 11.0656  |
|      |       | 40  | 4.768       | 13.2650  | 7.2975      | 4.768    | 13.2671     | 7.3162   | 4.808       | 13.0090  |
| Cs   | 5.63  | 2   | 5.096       | 0.6123   | 0.3494      | 5.096    | 0.6123      | 0.3494   | 5.109       | 0.5624   |
|      |       | 8   | 5.261       | 2.3990   | 1.3322      | 5.261    | 2.3994      | 1.3363   | 5.342       | 2.2918   |
|      |       | 18  | 5.390       | 5.3547   | 2.9775      | 5.390    | 5.3564      | 2.9963   | 5.443       | 5.1842   |
|      |       | 20  | 5.366       | 5.9403   | 3.2589      | 5.366    | 5.9414      | 3.2701   | 5.425       | 5.7729   |
|      |       | 34  | 5.445       | 10.1156  | 5.6044      | 5.445    | 10.1200     | 5.6235   | 5.488       | 9.8599   |
|      |       | 40  | 5.428       | 11.8123  | 6.4416      | 5.428    | 11.8144     | 6.4598   | 5.472       | 11.5881  |

*Here, $N=18$ corresponds to Al$_6$ cluster and other $N$’s do not correspond to a real Al clusters.
TABLE II: The absolute values at equilibrium state of the highest occupied and lowest occupied Kohn-Sham eigenvalues in rydbergs are compared for KLI, OEP, x-LSDA, and LSDA schemes.

| Atom | N  | $-\varepsilon_L$ | $-\varepsilon_H$ | $-\varepsilon_L$ | $-\varepsilon_H$ | $-\varepsilon_L$ | $-\varepsilon_H$ | $-\varepsilon_L$ | $-\varepsilon_H$ |
|------|----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Al   | 2  | 0.8152          | 0.8152          | 0.8152          | 0.8152          | 0.4367          | 0.4367          | 0.3012          | 0.3012          |
|      | 8  | 1.1142          | 0.6714          | 1.1088          | 0.7113          | 0.8201          | 0.3919          | 0.8821          | 0.4605          |
|      | 18 | 1.1727          | 0.5007          | 1.1619          | 0.5429          | 0.9497          | 0.3310          | 1.0129          | 0.4009          |
|      | 20 | 1.1856          | 0.5000          | 1.1804          | 0.4993          | 0.9665          | 0.2964          | 1.0282          | 0.3622          |
|      | 34 | 1.2055          | 0.4826          | 1.1998          | 0.4789          | 1.0192          | 0.2939          | 1.0853          | 0.3649          |
|      | 40 | 1.2292          | 0.4490          | 1.2136          | 0.4450          | 1.0541          | 0.2761          | 1.0965          | 0.3401          |
| Li   | 2  | 0.4777          | 0.4777          | 0.4777          | 0.4777          | 0.2445          | 0.2445          | 0.2983          | 0.2983          |
|      | 8  | 0.5760          | 0.4157          | 0.5735          | 0.4158          | 0.3935          | 0.2383          | 0.4476          | 0.2937          |
|      | 18 | 0.5935          | 0.3601          | 0.5879          | 0.3591          | 0.4523          | 0.2179          | 0.5062          | 0.2738          |
|      | 20 | 0.5889          | 0.3221          | 0.5865          | 0.3228          | 0.4522          | 0.1893          | 0.5061          | 0.2423          |
|      | 34 | 0.6029          | 0.3282          | 0.5991          | 0.3258          | 0.4832          | 0.2055          | 0.5374          | 0.2620          |
|      | 40 | 0.5979          | 0.2971          | 0.5950          | 0.2960          | 0.4816          | 0.1832          | 0.5355          | 0.2366          |
| Na   | 2  | 0.3883          | 0.3883          | 0.3883          | 0.3883          | 0.1951          | 0.1951          | 0.2437          | 0.2437          |
|      | 8  | 0.4467          | 0.3406          | 0.4451          | 0.3408          | 0.2963          | 0.1936          | 0.3453          | 0.2434          |
|      | 18 | 0.4544          | 0.2989          | 0.4502          | 0.2981          | 0.3374          | 0.1805          | 0.3859          | 0.2308          |
|      | 20 | 0.4485          | 0.2672          | 0.4470          | 0.2682          | 0.3361          | 0.1565          | 0.3851          | 0.2042          |
|      | 34 | 0.4583          | 0.2750          | 0.4551          | 0.2730          | 0.3588          | 0.1728          | 0.4078          | 0.2236          |
|      | 40 | 0.4520          | 0.2480          | 0.4502          | 0.2477          | 0.3564          | 0.1534          | 0.4055          | 0.2017          |
| K    | 2  | 0.3100          | 0.3100          | 0.3100          | 0.3100          | 0.1526          | 0.1526          | 0.1957          | 0.1957          |
|      | 8  | 0.3408          | 0.2733          | 0.3396          | 0.2735          | 0.2188          | 0.1536          | 0.2622          | 0.1977          |
|      | 18 | 0.3416          | 0.2422          | 0.3385          | 0.2415          | 0.2463          | 0.1458          | 0.2894          | 0.1902          |
|      | 34 | 0.3419          | 0.2246          | 0.3393          | 0.2230          | 0.2607          | 0.1413          | 0.3042          | 0.1861          |
|      | 40 | 0.3355          | 0.2025          | 0.3346          | 0.2027          | 0.2585          | 0.1255          | 0.3023          | 0.1683          |
| Cs   | 2  | 0.2723          | 0.2723          | 0.2723          | 0.2723          | 0.1324          | 0.1324          | 0.1724          | 0.1724          |
|      | 8  | 0.2923          | 0.2405          | 0.2913          | 0.2406          | 0.1843          | 0.1343          | 0.2247          | 0.1752          |
|      | 18 | 0.2907          | 0.2141          | 0.2880          | 0.2134          | 0.2061          | 0.1285          | 0.2461          | 0.1696          |
|      | 20 | 0.2850          | 0.1921          | 0.2847          | 0.1935          | 0.2048          | 0.1118          | 0.2454          | 0.1599          |
|      | 34 | 0.2897          | 0.1992          | 0.2873          | 0.1977          | 0.2176          | 0.1252          | 0.2580          | 0.1668          |
|      | 40 | 0.2835          | 0.1797          | 0.2831          | 0.1801          | 0.2157          | 0.1115          | 0.2564          | 0.1512          |