NONLOCAL STABILIZED JELLIUM CLUSTERS

N. Nafari
and
M. Payami

MIRAMARE-TRIESTE
ABSTRACT

We have used the stabilized spherical jellium model for the simple metal clusters (2 \leq N \leq 1106), i.e., Li, Na and K and have solved the Kohn-Sham equations self-consistently. The comparison of the local and nonlocal density approximations shows an appreciable difference between the total cluster-energies per atom for small size clusters. The magnitudes of these local-nonlocal energy differences in the case of the simple spherical jellium model are greater than the deformation energy differences brought about by the application of the ellipsoidal jellium model. The calculated binding energies for the stabilized spherical jellium model, in the limit of large cluster sizes, are close to the value of the bulk experimental binding energy of the corresponding metal. This is to be contrasted with the simple jellium model binding energy which is nearly three times smaller. The ionization potentials remain more or less the same for the local and nonlocal approximations and approach the bulk metal work functions.

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I. INTRODUCTION

In recent years, several authors have investigated the properties of metal clusters experimentally and theoretically. For an up-to-date review, one can refer to the articles by W. A. de Heer,¹ M. Brack² and the references therein. The theoretical studies often begin with the popular spherical jellium model (SJM) in which ions are replaced by a spherical uniform positive charge density of radius \( R = \frac{1}{3} \rho_s r_s \), \( Z \) being the total number of valence electrons and \( r_s \) being related to the bulk metal density, \( n \), through \( \frac{3}{4} \pi r_s^3 = n \) (all equations are expressed in Hartree atomic units).

The calculational scheme used to compute the ground state energy of metal clusters is often based on density functional theory (DFT) which has proved to be one of the most powerful techniques for understanding the energetics and electronic structure of inhomogeneous electron systems.

Thus, as the first step towards understanding the energetics of metal clusters, several workers, within the context of DFT, have used local density approximation (LDA) for SJM and solved the Kohn-Sham (KS) equations self-consistently.

Although, calculations based on SJM provide a vehicle for explaining the mass abundance spectra, the magic numbers of the clusters, and qualitatively predict the electronic excitations of these systems, but there appear several discrepancies between such calculated results and those of experiments. The roots of these discrepancies could predominantly lie (i) in the jellium model approximation (JMA) itself, (ii) in the use of the LDA in places where the density variations are large, (iii) in the assumed spherical symmetry and (iv) in any combinations thereof.

Let us consider these issues one by one. Firstly, from the work of Lang and Kohn (LK),³ it is known that JMA yields negative surface energies at high electron densities, \( r_s \leq 2 \). Also, as Ashcroft and Langreth⁴ have shown, the jellium bulk modulus for \( r_s \approx 6 \) is negative. Since the jellium cluster is the finite size version of the semi-infinite metallic jellium used by LK, the same drawbacks of JMA must show up in here too. The ionization potentials (IP) and the electron affinities (EA) predicted by SJM for Na and K are on the average too large. This is consistent with the result of LK for bulk work functions.⁵ There are different methods of rectifying the shortcomings of the simple JMA. One of the ways is to abandon the jellium picture altogether and include the ionic structure through pseudopotentials. This can be done either perturbatively⁶ or variationally.⁷ Also, the molecular dynamics methods in which the classical motion of ions is coupled to the quantum mechanical KS-equations for electrons,¹⁰ provide a good understanding of the energetics of these systems.

However, these methods are computationally very expensive and are suited for small clusters. Because of the simplicity of JMA and its low computational costs, some authors have tried to modify it in such a way as to keep its simplicity and yet avoid the above mentioned drawbacks. Perdew, Tran and Smith¹¹ as well as Shore and Rose¹² have pointed out that the failure of JMA arises because jellium is not in mechanical equilibrium. They, by introducing a structureless pseudopotential or pseudojellium, which forces the system to be mechanically stable, obtain surface energies, bulk modulus and cohesive energies in agreement with experiment. Recently, Brajczewska, Fiolhais and Perdew¹³ and Zicsche et al.¹⁴ have used the stabilized spherical jellium model (SSJM) to calculate various physical quantities of small clusters or voids. Our work in this paper starts with SSJM.

As mentioned before, there are other reasons for the discrepancies between the calculated results based on SJM and those of experiments. The LDA is expected to work well when the electron density variation over the characteristic length of the system is small. However, metal cluster densities near their surfaces, particularly for small cluster sizes, vary steeply. Moreover, the exact asymptotic behavior of the exchange-correlation (XC) energy densities, \( \epsilon_{xc} \), and XC-potentials, \( v_{xc} \), in finite systems are known to vary as \(-1/2r\) and \(-1/r\) respectively. This is contrary to the LDA incorrect predictions for which both \( \epsilon_{xc}(r) \) and \( v_{xc}(r) \) decay exponentially as \( r \to \infty \). Thus, it is imperative to go beyond LDA, particularly, when the ratio of surface atoms to the cluster size number, \( N \), is close to one.¹⁵,¹⁶ We will discuss the nonlocal density approximations (NLDA) used in this paper below.

Lastly, we could question the assumption of sphericity in SJM. To begin with, it is known
that the small size clusters tend to be planar. Moreover, from the analogous situations in nuclei, one expects the clusters having partially filled shells to be deformed. In other words, the spherical symmetry is an idealization which may ignore the fine structures stemming from the geometrical shape of the clusters.

Some researchers, having recognized the importance of nonspherical symmetry, have considered spheroidal or ellipsoidal jellium geometry and solved the KS-equations self-consistently. Naturally, certain technical problems arise in the use of the deformed jellium model. Firstly, the background jellium potential does not have a simple analytic form as in the case of SJM. Secondly, the KS-equations appear in two or three spatial dimensions which make the calculations more time consuming.

However, despite the technical difficulties, these authors have solved the KS-equations and obtained an appreciable decrease in energy per particle as compared with SJM. Their results, to some extent, explain the fine structures seen in the mass abundance spectra such as the relative energy per particle of the sodium clusters with atomic numbers of 34 and 40.

In this paper, firstly we have used the SSJM and secondly, the following two nonlocal exchange-correlation energy functionals (XCEF): (i) The modified weighted density approximation (MWDA) proposed by Gunnarsson and Jones and later on extended by Chacón and Tarazona. The form of the XCEF in MWDA is chosen in such a way as to fulfill the XC-hole sum rule at any given point r, and to reproduce the correct XC-energy density in the homogeneous limit. On the other hand, the Becke's proposed gradient corrected exchange-energy density functional is based on the fact that the major part of the error in the LDA-XCEF of a typical atomic or molecular system is due to the exchange energy density and this functional reproduces the correct $-1/2r$ asymptotic behavior for XC-energy density. As we have expected the use of these nonlocal functionals along with the stabilization of the jellium model has yielded results in closer agreement with experiment. To be consistent with the assumed spherical symmetry of SSJM, we have only considered the closed shell clusters in this paper. As the work of Clemenger for ellipsoidal jellium model shows the closed shell cluster energies assume their minimum when cluster geometry becomes spherical.

Here, we have solved the KS-equations of SSJM using the above-mentioned nonlocal functionals and have calculated the total energy per atom for lithium, sodium, and potassium clusters with $2 \leq N \leq 1106$. We have also calculated the IPs of these metal clusters. The comparison of our calculated results with the simple jellium model based on LDA shows significant improvements in the total energy per atom. But, the IPs remain more or less the same for local and nonlocal density approximation. Furthermore, the IPs asymptotically approach the value of the bulk metal work function with increasing N. The preliminary results of our work for the simple spherical jellium model were presented in Ref. 15.

The organization of the paper is as follows: In the second section we present the calculational schemes. The third section is devoted to the results of the calculational schemes of LDA, MWDA, and BGCA for the total ground state energy per atom and the IPs for closed shell stabilized jellium clusters. Finally, the fourth section concludes this work.

II. CALCULATIONAL SCHEMES

In the stabilized jellium model, the total ground state energy of a metal cluster with positive background of density $n_+(r)$, as a functional of electron density, $n(r)$, is given as

$$E_{\text{tot}}[n] = E_{\text{ion}}[n] + (\varepsilon_M + \omega_R) \int n_+(r) \, dr,$$

where $n_+(r) = n\Theta(r)$, with

$$\Theta(r) = \begin{cases} 1 & \text{for } r \leq R \\ 0 & \text{otherwise} \end{cases}$$

and $R$ is the radius of the jellium sphere. $\omega_R$ is the average of the repulsive short-range part of the pseudopotential and $\varepsilon_M$ is the average Madelung energy over the Wigner-Seitz cell of a collection of point ions embedded in a uniform negative background of density $n$. $(\delta \varepsilon)_{WS}$
The jellium energy functional is
\[ E_{\text{Jell}}[n, n_+; r] = T[n] + E_{\text{ex}}[n] + \frac{1}{2} \int \phi[n, n_+; r] \left[ n(r) - n_+(r) \right] dr, \]
where
\[ \phi[n, n_+; r] = \int \frac{n(r) - n_+(r')}{|r - r'|} dr'. \]

To evaluate the total energy of a stabilized cluster, we solve the KS-equations,
\[ \left[ -\frac{1}{2} \nabla^2 + v_{\text{eff}}(r) \right] \psi(r) = \epsilon \psi(r), \]
self-consistently. Here the effective potential, \( v_{\text{eff}}(r) \), is
\[ v_{\text{eff}}(r) = \phi[n, n_+; r] + v_r + (\partial \phi)\omega x \Theta(r), \]
and the ground state electron density, \( n(r) \), is evaluated using the \( N \) lowest occupied KS-single particle orbitals, i.e.,
\[ n(r) = \sum_{i=1}^{N} |\psi_i(r)|^2. \]
The XC-potential, \( v_{\text{xc}}(r) \), contains all the many-body effects not contained in the classical potential, \( \psi \), and is by definition equal to the density variation of the XCEF, i.e.,
\[ v_{\text{xc}}(r) = \frac{\delta E_{\text{xc}}[n]}{\delta n(r)}. \]

In the following subsections, we specify the form of the XCEF appearing in the MWDA and the BGCA.

**A. The MWDA scheme**

In this scheme one starts with the exact relation between the XCEF and the pair-correlation factor, \( G(r, r') \), i.e.,
\[ E_{\text{xc}}[n] = \frac{1}{2} \int \frac{n(r)n(r')}{|r - r'|} G(r, r') \, dr \, dr'. \]

\( G(r, r') \) is given in terms of the pair-correlation function \( g_s(r, r'; n) \) with \( \lambda \) as the strength of the interaction between particles, i.e.,
\[ G(r, r') = \int_0^1 \left[ g_s(r, r'; n) - 1 \right] d\lambda. \]

It is well known that the exact asymptotic behaviors of the XC-energy density, \( \epsilon_{\text{xc}} \), and the XC-potential, \( v_{\text{xc}} \), in finite systems are respectively \(-1/2r\) and \(-1/r\), in contrast to the LDA results for which these quantities decay exponentially.

It has been suggested by Gunnarsson and Jones\(^1\) to use the following analytic form for the pair-correlation factor, \( G(r, r') \),
\[ G(r, r') = C \left( 1 - e^{-\frac{r^2}{\lambda^2}} \right). \]

For a given value of \( n \), the parameters \( C \) and \( \lambda \) can be determined through the following two equations in the homogeneous limit,
\[ \frac{1}{2} \int \frac{G(r, r')}{|r - r'|} \, dr' = c_{\text{xc}}^0(n), \]
\[ n \int G(r, r') \, dr' = -1. \]
\( c_{\text{xc}}^0(n) \) is the XC-energy density for the homogeneous electron gas at the given density \( n \) and Eq. (13) is the XC-hole sum rule in that limit. For a non-uniform system, the values of \( n \) depend on \( r \), and is determined at each point by the requirement that the XC-hole normalization sum rule must be satisfied, namely,
\[ \int n_+(r, r') \, dr' = \int G(r, r')n(r') \, dr' = -1. \]

The fulfillment of this equation at each point \( r \), defines \( n(r) \), and thereby the expression for \( G(r, r') \) takes the assumed form of \( G( |r - r'|, n(r)) \). By performing the variation of \( E_{\text{xc}}[n] \) with respect to \( n(r) \), one finds the following expression for \( v_{\text{xc}}(r) \):
\[ v_{\alpha}(r) = \frac{\delta E_{\alpha}[n]}{\delta n(r)} = v_1(r) + v_2(r), \quad (15) \]

where \( v_1(r) \) and \( v_2(r) \) are given by:

\[ v_1(r) = \frac{1}{2} \int \frac{n(r')}{|r - r'|} G(|r - r'|; n(r')) \, dr', \quad (16) \]

\[ v_2(r) = \frac{1}{2} \int \frac{n(r')}{|r - r'|} \delta G(|r - r'|; n(r')) \, dr', \quad (17) \]

As Gunnarsson, Jonson and Lundqvist\(^25\) discuss, the resulting \( v_{\alpha}(r) \) and \( v_x(r) \) have the same asymptotic behaviors of \(-1/2r\), which is an improvement over LDA. The spurious factor of \(1/2\) in the asymptotic behavior of \( v_{x}^{\text{WDA}}(r) \) arises from the fact that this \( G(|r - r'|; n(r')) \), in contrast to the symmetry property of the exact \( G \), is not symmetric in \( r \) and \( r' \).\(^26\) The expressions for \( v_1 \), \( v_2 \), and \( v_x \) in the case of spherical symmetry have been calculated by Ossicini and Bertoni\(^27\) and will not be reproduced in here.

### B. The BGCA scheme

In general, one may write any gradient corrected exchange energy density functional as:

\[ E_{\alpha}[n_1, n_2] = -\frac{3}{2} \int r 3 \left( \frac{3}{4\pi} \right)^{1/3} \left( n^{4/3} + n^{4/3}_2 \right) \, dr + F_x [n_1, n_2, \nabla n_1, \nabla n_2, \ldots], \quad (19) \]

where \( n_1 \) and \( n_2 \) are the spin up/down densities, and \( F_x \) is a functional with certain properties. The Becke's proposed expression for \( F_x \) is:

\[ F_x [n_1, n_2, \nabla n_1, \nabla n_2, \ldots] = -b \sum_{\sigma=\uparrow, \downarrow} \int n^2/2 Q(x_\sigma) \, dr, \quad (20) \]

where \( x_\sigma = |\nabla n_\sigma| \left/ n^{2/3}_\sigma \right. \), and

\[ Q(x_\sigma) = \frac{x^2_{\sigma}}{1 + 6b \sigma x_{\sigma} \sinh^{-1} x_{\sigma} \right. \quad (21) \]

The value of the parameter \( b \) entering the expression for \( F_x \) is determined by a fit to the atomic Hartree-Fock data and turns out to be 0.0042 in Hartree atomic units. The exchange potential to be used in our self-consistent calculations is:

\[ v_x = \frac{\delta E_x}{\delta n} = -\frac{4}{3} \left( \frac{3}{4\pi} \right)^{1/3} n^{4/3}_x + b n^{2/3}_x Q(x_\sigma) - \frac{b}{|\nabla n_\sigma|} \left( \frac{dQ}{dx_\sigma} \right) \]

\[ + \delta x_\sigma \left[ \frac{\nabla n_\sigma}{|\nabla n_\sigma|} \frac{dQ}{dx_\sigma} \right], \quad (22) \]

For the correlation we employ the Vosko, Wilk and Nusair\(^28\) parametrization of the Ceperley-Alder's results of the Green's function Monte-Carlo data.\(^29\) The Becke's gradient corrected functional reproduces the proper asymptotic behavior for the exchange-energy density, i.e., \(-1/2r\). Moreover, although the XG-potential in here, instead of showing the correct asymptotic behavior of \(-1/r\), goes proportionally like \(-1/r^2\),\(^30\) it is yet behaving somewhat better than \( v^{\text{LDA}}_x \).

### III. RESULTS

In this section we present our calculated results for the simple metal clusters \((2 \leq N \leq 1106)\), i.e., for Li, Na and K. In our calculations for closed-shell clusters, the \( r_s \)-values for Li, Na and K are chosen to be 3.25, 3.93 and -1.86 respectively.\(^32\) After computing the wave functions and the eigenvalues, the total energy of an \( N \)-atom cluster, \( \epsilon^{(N)} \), were calculated for \( N = 2, 8, 18, 20, 34, 40, 58, 68, 92, 268, 476, 1106 \). Figs. 1(a), 2(a) and 3(a) show the plot of \(-\epsilon^{(N)}/N\) as a function of cluster size, \( N \), for Li, Na and K respectively. The calculations are performed for the stabilized spherical jellium model along with the BGOA scheme. Figs. 1(b), 2(b) and 3(b) are the counterparts of Figs. 1(a), 2(a) and 3(a) using the simple spherical jellium model. Next, for the sake of comparison, we show in Fig. 4(a) the same calculation of \(-\epsilon^{(N)}/N\) for Na using SSJM with the three calculational schemes of LDA, MWDA and BGCA. Fig. 4(b) is the counterpart of Fig. 4(a) using the simple spherical jellium model. These plots show oscillations in the value of the total cluster energy per atom. The amplitudes of these oscillations become smaller with increasing \( N \), and the energy reduces to a constant.
value in the limit of large N. Such expected behaviors in the limit of large cluster sizes are the signature of bulk properties. Furthermore, there is a significant difference between the calculated $E(N)/N$ for small size clusters when LDA versus NLDAs are used. As Fig. 4(a) shows, this difference decreases with increasing N. This is because, small clusters have large electron density variations throughout their systems, whereas the large size clusters have steep density variations only near their surfaces. Had we used the more appropriate ellipsoidal geometry for small clusters, the greater inhomogeneity of the system would have given rise to an even greater difference between the local and nonlocal calculations. These plots, in particular Figs. 1(a), 2(a) and 3(a) show that our calculated large cluster binding energies using SSJM are close to the experimental bulk binding energies of the corresponding metal. The experimental binding energies of Li, Na and K are respectively 7.02eV, 6.25eV and 5.28eV and the binding energies of the 1106-atom clusters are respectively 7.80 eV, 6.35 eV and 5.09 eV. On the other hand, as shown in Figs. 1(b), 2(b) and 3(b), the binding energies of large size simple jellium clusters along with the BGOA calculational scheme turn out to be about 2.0 eV. Consequently, the SSJM has greatly improved the values of the SJM binding energies.

We, furthermore, observe that the difference between the calculated binding energies of the two models (SSJM and SJM) for sodium clusters appear to be a simple shift for all cluster sizes. This is because of the fact that the sodium r, value ($r_s = 3.93$) is very close to that of the stable jellium ($r_s = 4.2$). So, the effect of the difference potential, $\delta\phi(r)$, is not so important for sodium. However, the self-energy correction remains valuable and it is the effect of this correction which appears roughly as a shift in the binding energies.

Finally, the positions of the broad peak in Figs. 4(a) and 4(b) for NLDAs give a rough estimate of the cluster sizes for which the bulk properties begin to set in. A rough calculation shows that beyond the approximate positions of these peaks ($N \approx 100$ for Li, $N \approx 200$ for Na and $N \approx 400$ for K), the number of surface atoms becomes smaller than the number of interior ones.

Fig. 5 shows the ionization potential energies of an $N$-atom sodium cluster defined as the difference between the total energy of that system with $Z$ and $(Z-1)$ electrons. The calculation of IPs are performed for the SSJM with the aid of LDA and NLDAs mentioned in this paper. As seen in this figure, the value of the IPs for large-N clusters tend to the value of the work function of the bulk sodium, i.e., 2.35 eV. There is not much of a difference between the IPs of the two jellium models (SSJM and SJM) and the agreement between these results and experiments are not satisfactory. This is also true for lithium and potassium. The reason are two-folds. Firstly, since IPs are, by definition, the difference of two total energies, their accuracies are somewhat less than that of the total energies. This entails that the SSJM improvement of the total cluster energies has not been sufficient for obtaining reasonable estimates of cluster IPs. Secondly, one should not expect the spherical jellium model calculations show the observed fine structures of IPs. In fact, in order to produce the odd-even alternation effect theoretically, one has to break the spherical symmetry and introduce nonspherical models.

In Fig. 6, we plot the XC-potentials using the above-mentioned three calculational schemes for the typical sodium cluster with $N = 476$ as a function of radial distance r. The interior part of the BGCA-XC-potential shows oscillations with larger amplitudes relative to the other two cases. Since LDA-XC-potential decays exponentially and the asymptotic behaviors of the MWDA- and BGCA-XC-potentials are proportional to $-1/r$ and $-1/r^2$ respectively, the tail of the BGCA curve, as expected, lies between the other two potentials.

Fig. 7 shows the plot of the electron density as a function of r for Na$_{476}$ cluster. Here again, we observe relatively sharp oscillations for the BGCA case, and their behaviors outside the clusters are more or less the same.

IV. CONCLUSION

In this paper we have modeled our metal clusters as an stabilized spherical jellium which is known to rectify the anomalies of the simple jellium. The often employed LDA works well when the electron density variation is slow. However, since the variation of the electron
density near the surface of a cluster is steep, one needs to go beyond LDA and we necessarily used various nonlocal density approximations as described in this paper. Because of the greater inhomogeneity of the small size clusters, the difference between the results of LDA and NLDA's for total energies per atom, as seen in Figs. 4(a), 4(b), is quite appreciable. The importance of these local-nonlocal energy differences for small size clusters are better seen when they are compared with the deformation energy differences (defined as the difference between the total cluster energy per electron for the ellipsoidal and spherical jellium model using LDA).

The self-consistent triaxial results of Hirschmann, Meyer and Brack\textsuperscript{36} (also see Fig. 3 of Ref. 2), as well as the triaxial results of Yannouleas and Landman\textsuperscript{35} show maximum deformation energy difference of about 0.07 eV for clusters of size $8 \leq N \leq 20$, whereas our spin-compensated local-nonlocal energy differences for the same clusters, as seen in our Fig. 1 of Ref. 15 is about 0.25 eV. In other words, for small size clusters, the effects of nonlocality are greater than the effects of geometry. Thus, in any quantitative calculations of cluster binding energies, one must include the nonlocal and geometrical effects simultaneously. However, if one is interested in the calculation of the ionization potentials, the geometry plays an important role. This is because the calculation of the IPs involves the difference between the total energies of the system with $Z$ and $(Z - 1)$ electrons. The local-nonlocal energy differences of the two systems with $Z$ and $(Z - 1)$ electrons are very close for open shells, whereas the deformation energy differences are appreciable. For clarification purposes, let us mention that consistent with the nonspherical electronic charge distribution of the open-shell structures, one assumes nonspherical geometry for the jellium positive background. This, in turn, lifts the spherical degeneracy and splits the spherical shells into subshells. From the filling of the subshells with even number of electrons one can easily explain the reasons for the well-known odd-even alternations in the metal cluster IPs. Since, on the one hand, accounting for nonlocality in the stabilized jellium model has given better binding energies, and on the other hand, the inclusion of nonspherical geometry has opened a way of explaining the odd-even alternations of IPs, we expect to obtain better agreement with experiments, when both effects are taken into account.

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REFERENCES


32 In order to be consistent with our zero-temperature KS-equations we have used the zero-temperature \( r_s \) values. The room temperature \( r_s \) values are slightly larger (less than two per cent) and will produce slight changes in the calculated total energies per atom.
FIGURES

FIG. 1. Absolute value of the Li-clusters total energy per atom, \(-E(N)/N\), in units of eV as a function of cluster size, \(N\), with the nonlocal calculational scheme of BGCA for (a) the stabilized spherical jellium model, and (b) the simple spherical jellium model.

FIG. 2. Absolute value of the Na-clusters total energy per atom, \(-E(N)/N\), as specified in Fig. 1.

FIG. 3. Absolute value of the K-clusters total energy per atom, \(-E(N)/N\), as specified in Fig. 1.

FIG. 4. Absolute value of the Na-clusters total energy per atom, \(-E(N)/N\), in units of eV as a function of cluster size, \(N\), for (a) the stabilized spherical jellium model, and (b) the simple spherical jellium model. The results of the three calculational schemes of LDA, BGCA, and MWDA are shown by diamonds, plus signs and squares respectively. The differences between the local and nonlocal energies for small clusters are appreciable and decrease with increasing \(N\). Note that the calculated binding energies of the large size stabilized cluster for the three calculational schemes of LDA, BGCA and MWDA are close to the bulk experimental value of 6.25 eV.

FIG. 5. The ionization potentials of Na-clusters in units of eV as a function of cluster size, \(N\). The calculations are performed for the three schemes of LDA, MWDA, and BGCA using the stabilized jellium model.

FIG. 6. The XC-potentials in units of Rydberg as a function of the radial distance, \(r\), in atomic units for Na476 cluster. The dotted, dashed, and solid lines correspond to the LDA, MWDA and BGCA calculational schemes respectively. The BGCA-XC-potential yields stronger oscillatory behavior.

FIG. 7. Electron density in atomic units as a function of radial distance, \(r\), for Na476 cluster. As in Fig. 6, the BGCA calculational scheme, in comparison with the LDA and MWDA, results in stronger oscillatory behavior.


(a) Stabilized-Lithium

Fig. 1(a)

(b) Simple jellium-Lithium

Fig. 1(b)
Fig. 2(a) Stabilized-Sodium

Cluster size N

Fig. 2(b) Simple jellium-Sodium

Cluster size N
Fig. 5

Fig. 6

Sodium

Fig. 5

Fig. 6
Na-476

Fig. 7