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SFI5869 - Técnicas de escrita científica em inglês

DFThesaurus

based on Density-functional theory papers

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VII) Acknowledgements

- *support*
- *helpful discussions*
- *computer resources*

I) Abstract

* In DFT papers, the purpose is the most common start for an abstract. Nonetheless, here we give some suggestions for background and gap, which can be joined to the suggestions of the introduction section.

1. Background

different ways of setting a scenary

In electronic many-particle systems, ...
An old and yet unsolved problem in ... is ... . This arises from the fact that ...
A scheme that reduces the calculations of ... has obvious advantages. It is not surprising, then, that the ... has received much attention in the past ... .
The calculation of ... is a sensitive test of ... in ...
Consider a system with a ... constraint on its ... (e.g., that there are ...). We show that ...

bringing on a technique

Having been widely used for (over) ...
... it has more recently also become popular with...
... calculations, mainly using the ... approximation, have been used to investigate the ... on ....

exposing an interesting feature of sth

These models are designed to be ...
The presence of ... enables ... to ...
The ... embodies ...
... is known to be ...
... is known to satisfy ...
... which has fundamental and ... implications for ...

2. Gap

Despite the remarkable ... (accuracy of) ... with the ...
Unlike conventional ...
Unlike previous work in this area ... we focus on ...
..., but ... are not.
... is approaching an impasse. To continue to progress toward the ...
Whereas conventional ... cannot describe ..., ... is shown to do all well.
The well known ... gives excellent ..., but seriously overestimates ...

3. Purpose

We describe our attempts to improve upon the quality of ... through ... . A ... is presented , which ...
We study the.. / We present ...
This paper studies the ...
In the present paper/study ...
In this ..., the authors survey the formalism and some of its applications ... and discuss ...
The present article is directed at ...
It aims to convey the...
.. is/are discovered, ...

... discussed and illustrated.
The application of ... to ... and ... properties is discussed within the ... .
A ... is presented, which maintains the ...
This problem is solved in the present paper by ...
Therefore, we have investigated the ...

4. Results

- statement of results (=what was done?)
We demonstrate that ...
We have constructed a ...
We support the idea that ...
We consider the ... correction term of ...
We also discuss...
We present results on the ... and ... .
We illustrate our results with ...
We derive a method to calculate the ... of the ... .
For the extensive range of systems considered in this study, ... provides ...
Furthermore, this is accomplished within a ... procedure that ...
We introduce an (efficient/self-consistent) ... based on ... , and compare the performance of ... .
... are described, particularly their use in reducing the computational effort required.
We discuss the implementation in ..., and how ... calculations may be efficiently performed on ....
In fact, we obtain accuracy that ...
We show that in ... theory, the ... consistent with the constraint is actually a ..., and that this solution is unique. This leads us to an efficient algorithm for calculations on constrained systems.
Illustrative studies are shown for ...
We show that ... is size-consistent: one obtains the correct ... when the ... .
We also study a model ..., where experiments suggest a ... .

On ... the results for ..., in particular, were sensitive to the ... functional used in the calculations, but in all cases failed to reproduce the experimentally-established ...
This result is discussed in the context of previously published ... results for these ... .

- good results
Significant improvements over the ... are obtained in ...
This ... performs significantly better than ...
We find systematic improvements,
... qualitative as well as quantitative,
... that are as accurate as those from the best ...
... provides ... that are comparable to, (or that surpass,) those of the ... (best present-day) ... .
Excellent agreement is found between theory and experiment within the ... .
The optimal geometry found for ... is similar to that on ..., providing agreement with experiment regarding the ...
For ... distances, ... also correctly describes the ... dependence of the ... on the ... .
With an appropriate model, we obtain qualitative agreement with experiments and estimate the ... .

- problems
... most of the error of ... for ... arises in the description of ..., by ...

On ... the results for ..., but in all cases failed to reproduce the experimentally-established ...

5. Experimental
We apply the ... and show that it properly ...
In our approach, the constrained state is calculated directly by ... .
Here, we show that the same ... approach applies to systems with ... .
To illustrate the utility of this approach, we focus on the study of ... .
... is used to explicitly calculate the ... curves of both the ... and the ... .

6. Conclusion
We find that ...
We also discuss the ...
We suggest that ...
... can lead to further progress.
Thus the (numerous/well-known) problems of ... are circumvented.
Further improvements are required in the ...

II) Introduction

1. Background

importance of this issue
The development of new ... is an essential aspect of ... . Many ... have been developed, ... At present, the vast majority of ... use ... .
The study of ... systems is one of the central issues in the ... . Examples are ...
In view of the ... (eg. prominent) role ... plays in the ... it is a worthwhile endeavour to ...

time evolution of this matter
In recent years, ...
Since ... birth, ... has become ...
Over the past ... years, ...
... has become the most commonly used methodology of calculating accurately the physical properties of a vast range of materials.
... can now achieve accuracy in the order of ... . The best tested theories have ...

introducing the general idea/formulation of the method
In its usual formulation, ...
The starting point of ... is ...
..., particularly in the version pioneered by ..., has become very popular in ... .
... . Being a ... method it exhibits many of the advantages of the conceptually important ... , but incorporates ... .

emphasizing the role of ...
... is widely used for ...
... is one of not many...
... strive to improve upon the ...
... extends the scope of the ... to allow the *ab initio* calculation of ...

reviewing previous work
... is a remarkable result due to ...
A recent study ... shows that ...
Recent developments concentrate on ...
In a previous study, ... determined ...
Significant advances in the formalism of ... were made by ... . The developments introduced in those seminal papers showed that ...
The ... formulation of ... due to ... is particularly elegant.
A very similar formula was presented by ... .
... and ... presented a formula where ... is given not as the ... but as a ... . However, they did not show how to treat ... .

2. Gap
It is, however, ...
On the other hand ...
As with the ... , however, the model does not capture the ...
However, progress in ... requires ... (capability to deal with ...)
Traditional methods are ... (well suited) for ... . However, ... imposes rather strict limits on ...
... techniques are powerful aids, but do not work in ..., and are not easy to apply in ...
The ... can, in principle, be applied to ..., but neglect ...
... makes it unreliable as a tool for studying ... (many issues of current physical interest in ...)
Note that ...
To make progress in ..., ... are required.
The last problem (illustrates) a fact that is ... (often) (overlooked)
... involves ... . Unfortunately, the ... calculations are problematic. First of all, ... may not be ... . cannot be handled by ... .
Even in ... cases to which ... should apply, however, ... difficulty may arise. These are cases where ...
There are several reasons, however, why it is desirable to continue to develop ... . First, it is of theoretical interest to ... . Second, ... A notable example is ... . Third, ... And finally, ...
It is sometimes possible to calculate ... using a ... approach to obtain the ... . However this method fails when ... . Obtaining ... motivated the developments ... which is able to treat an ... .
... and ... presented a formula where ... is given not as the ... but as a ... . However, they did not show how to treat ... .

3. Stating the purpose
The present ... is mostly concerned with the ...
In this paper we shall first ... Next, ... Finally, ...
This article is aimed (primarily) at ...
We have implemented ... for ... using ...
In this paper we will describe developments of the theory and implementation of ...
In particular we give the formalism to compute ... in the ... for ... in a ... consistent manner.
We present an efficient ... for the ... .
We discuss the use of ... to optimize the number of ... calculations needed to obtain ...
Finally we will present some results of ... applied to ... .
We also benchmark against previous calculations where results are available to demonstrate the consistency of our implementation and methods.

4. Methodology

explaining a little about the technique
This ... interaction is introduced into ... by virtue of a ...
Within the ... approach ...
In this theory, ...
It is based upon the ... theorem which states that the ... response of the ... may be calculated using ...
It can be deduced that ... obey a ... principle, or for ... a ... .
This allows the method to be formulated as a problem of ... which may be solved using efficient algorithms such as ... .

positive aspects of the technique chosen
In ... calculations, ... provides a convenient and reliable way to ...
While .... is in principle ..., its pratical implementation requires the use of ...
These systems were chosen as they had been used previously in the development of the
Such a method provides ... (the computational and conceptual) advantages of a ... method but can, in principle, provide the ... results for the ... .
Hence, without all the formal and computational complications of ... methods such as ..., ... or ... ; a ... result, in principle, includes the ... .
The variational formalism has the inherent advantage that it is ... and does not require a ... .
Further, the computational cost is comparable to that of a ... , although there are further implications when ... is considered.

5. Concluding the introduction
In Sec. ... we describe the development of ...
In Sec. ... its performance is compared to that of ... .
Conclusions are presented in Sec. ...
All calculations use the ... program.

III) Model and methods *many times joined to results

1. A brief intro
In this section we compare the performance of ... with that of ... and ... for a range of ... . We also compare with the results from other ...
A key consideration during the development of ... was to maintain the ... . We therefore commence by investigating ...
The central task in any ... calculation is the construction of the ... . In the absence of ... other than the ... this requires ...
The central problem is to find a ... which ... . The prerequisite is ...
From a computational perspective the problem is to determine ... and the relationships between ...
A ... chain is the simplest possible model system resembling the ...

previous work
The theory of ... is discussed in detail in the review by ...
Our implementation is based on the ... scheme of ... and we use the same notation.
Our method for calculating ... begins from the work of ... who noted that ...
Previous work on ... has used a ... approach to calculate the ... . That approach can be problematic; in

particular ... . A ... approach is also more effective for ... which can require ... to converge a ... calculation.

giving examples
Notable examples include the calculation of ...
Examples are ...
A notable example is ...
... methods such as ...

2. Description of the procedure

- starting
We commenced from the ... in ... and investigated whether improved results could be obtained by ...
All calculations begin with ... as described below in a ...
Within the spirit of this ... approach, we ... / In this approach, ...
Our approach is similar to that of ... . is constructed to be ... while satisfying all of ... . This is accomplished by the following algorithm ...
Our method chooses an initial guess for the ... based on the previous iteration and scales it if necessary.
Neglecting spin, we construct a model based on ...
In the density-functional calculations for the ... we used a ...
Within the ... approximation, it follows that ...
Ultimately we intend to apply our method to ... . These are ...

- what is done?
The ... is minimized along this direction using a ... minimizer.
The ... is determined using the ... .
The first ..., denoted ..., was constrained to satisfy the ..., i.e., ..., with the remaining parameters, ..., determined by fitting to experimental ... data.
The ... used the same values of ..., ... and ... were determined through a fit to ... and ...
Both ... perturbations were calculated in order to evaluate both ... contributions to the ... .
The resulting ... as a function of ... was subsequently approximated through the first terms in a ... expansion:
The ... for the ... calculations is given by the difference of the ...

- verbal explanation
We compared ... forms of the ... function: ...
We assume ... for simplicity.
We optimized the geometries of the ...
We approximate ... as follows: ...
We investigated a number of ...
We followed accordingly ... different approaches for obtaining the ... parameters from the results of the ... calculations.
We now apply the functional to the determination of some properties of the ...
In our calculations, we determine the ...

- general description
We investigated a number of different ... : that of ... , the modification due to ... , and one due to ... that was specifically designed for use in ... applications.

We use a more general approach ... which is to compute ... . Further to this, we make use of the ... to reduce the computational cost which we describe in detail, below.
We obtain the ... using a ... . Our method varies the coefficients of ... simultaneously using a method similar to ...
We examine the ... through ... . Only ... need to be considered.
A very similar analysis is performed to establish the ...
For this ... case a ... was used to sample the ...
We start with an initial guess for the ... , which allows us to calculate the ... This gives in turn a new set of ... .
This procedure is repeated until self-consistency is achieved.

- details of the procedure
We let the energy zero be at ... and introduce ... Furthermore, we assume that ... Then ...
Applying ... boundary conditions to a ... chain with ..., the can be written as ...
Assuming that for each ... there are ..., we obtain ...
Scaling the .. for the ..., one obtains ...
For large chains, the properties of ... can be calculated using the method that allows reliable ... to the ...

From these we can calculate the elements of the ... via ...
Finally, in the absence of ... , ... implies ...

- how?
Our/all calculations ... are/were performed within (DFT) ... for the ...
Our/all calculations on ... were performed (self-consistently) using ...
For ... , we used the theoretical estimate ...
The ... was used to describe the ... interactions and a ... optimization was performed to ...
In the density-functional calculations for the ... , we used a ...

- why?
In order to extract the ... from ...
In order to determine the ..., we performed model calculations with the same set of ...
In order to analyse our results, we define a ... via ... where ...
In order to perform ... calculations, we fitted the ...
In order to derive a ... for this system, we follow ... and express the excess (over ideal) ... as a ...
To obtain an accurate location of the ... in a ... requires that the ... .
To avoid oscillations we had to apply a ...
To this aim we expand...
For the present purposes, it is convenient to cast ... in the form ...
For the sake of comparison, we therefore performed calculations with the same values of ...
A ... is unnecessary because ... .
... thus further increasing the speed of the ... .
We use therefore in addition the experimental value of the ...
Another modification is required, however, to ...

3. More about the method
We use the model constructed by ... in their study of ... , since ...
The other route, which we pursue here, is based on the ... relations.
The theory of the application of ... to ... was set out by ... using the ... .They showed that ...
The ... model was motivated by the ... as a ... . It reproduces, by construction, the ... . In any other

system, it is an approximation to ... .
This method uses more memory than ... ; however, the computational time is considerably lower because only one ... is required per ... cycle.

important remarks

This number may be reduced by a large factor by exploiting the ...
The ... poses no fundamental problem ...
For the present purposes, notice that the ..., like the ..., is ... and has a ... .
Note that this will lead to different values of ... in the ... and the exact calculations.
In our experience, ... requires about the same computer time as ... on most machines.
A further consequence of the ... is to fix the ...
A simplified version of the algorithm used for the ...is used to avoid unnecessary recomputation.
In contrast to the case for ... , we are not able to obtain exact solutions for the ... chain.
In the absence of ... this corresponds to having only ...
It is very important to note that ... is fairly independent (within ...% from the mean value) of the ...
It is important to remark that ...
Notice that ... preserves the previous general properties ... and that it is of course exact for ...

some practical details

Our set test includes/(makes use of the) ...
The ... comprised the vast majority of the standard ... set, together with the ...
Experimental values of ... were taken from ...
The ... were set equal to ...
These conditions are satisfied to a high degree of numerical precision and are easily identifiable from the ...
In practice, the ... can be easily obtained by ...
Only ... are considered since this is the relevant domain when all the ... have the ... .

further information

... has been/is described in ... (detail) ...
Comparative plots of the ... may be found in Ref. ... . The model is sufficiently flexible to ...
We can also treat ... and related properties from consideration of the ... in direct analogy with that of ..., except we have to use the ...
In addition to the ... so far discussed, it is possible in some ... to ....
A very similar analysis is performed to establish ... . These resemble those of the ... with the difference that ...

other approaches

Alternatively, ... with ... can use the approach of ..., (which we have followed here.)
The approach of ... is to make use of ... computed during the ... procedure which ...
Our analysis goes further than that of ... in detecting ... . This is achieved by repeating the analysis with a new initial ... generated using ...

describing equations

The simplest approximation for the ... reads
The ... then takes the form ...
In other terms, ... has the form ...
Indeed, the ... is given by ... .
Then, setting x = ..., simultaneous solution of Eqs. (...), (...) is achieved by solving the ... problem, ...

Then the ... and related properties such as the ... required to give ... come from ...
following which ... is obtained from ... and finally ... .
Equation (...) is easily solved, for all possible ... and ..., by the ... method.
Equation (...) applies to the ...
Using Eq. (...) it is straightforward to show that ...

IV) Results

1. "Introduction"

Our ... is characterized by the ... and ... .These parameters are coupled through ... Eq.(...), which implies ... .
Due to its simplicity, the ... is an excellent system on which to test new approaches, and therefore we will study it first.
Thermodynamically, the system can be characterized by the ...
In ... , ... was published. The model connects ... ... (in an elegant way), through ... and it treats ... .
Another feature is that ...

2. Reference to previous results

The ... is based on the ... (as a starting point). This distinguishes the ... from most others in the literature. It ... but does not ... . The result of our model is ...
We refer the reader to Ref. ... for details on solving ... and obtaining ... .
... has pointed out that ... . We find that ...
Following Ref. ..., we determined ... for the ... together with the ...
In Ref. ..., we observed that ...
These results agree with the observations stated in previous studies on ... regarding the ... and ... .
The theory of ... is discussed in detail in the review by ... . Our implementation is based on the scheme of ... and we use the same notation.

3. Statement of Results

- what results?

We have confirmed that ... differences from ... are very close to those of ... and ... .
We obtain a total ... from Eq.(...) of the form ... , where ...
We find that ... saves approximately ...% of the CPU time.
We have also examined the effect that the ... has on the molecule.

From the ... analysis, results show that ...
Least-squares fits for the three sets of calculations to equation (...) led to ...
For a ... , the ... fit of the ... yielded ...
It also demonstrates that the ... approximation may not be very good when ... becomes comparable to or larger than ... .
Analogous results are obtained for ... (not presented).
Finally the symmetry of ... is that of ...
As a result one recovers the phase diagram of ...
The ... almost coincide, except for ... at small ... .
In the most difficult ... case, we find ...
The largest discrepancies are found for ...

In all cases the quantitative differences remain small ...
The ... of over ... at first seems paradoxical, as it would appear to imply that ....
The ... diverges with the ...

- about performance
Once again, ... and ... are more accurate, with ... providing the best overall performance.
It surpasses ... and ..., giving essentially the same quality as ..., which arguably provides the highest quality ... of any ... .
The best performing ... was the original ... variant, despite being intended for a ...
The ... showed the worst performance despite being specifically designed for ... calculations. However, the differences between each are relatively small.
In both cases the ... and ... converge the ... at approximately the same rate.
Although the ... parameters are only slightly changed, showing the usual ... underestimation, the highest branch is increased in ... to a range of ... compared to ... using the ... .

- comments on errors
The ... mean absolute error ... is a significant improvement over ... and ... .
The mean absolute error from ... is slightly inferior to that of ... and ... , but remains a substantial improvement over all the other ...
Errors from ... are substantially larger.
Even the ... and... give larger errors.
... uniformly overestimate, with errors of ..., respectively.
... provide a good quality description, with mean absolute errors of ... .
A final point which merits a remark here is the very large error in the ... made by the ...

4. Figure

- introducing a figure
In Fig. ... we compare our results with those from the ... approximation for a given ... .
In Fig. ... we see that the fitted ... curve has a non vanishing offset.
In Fig. ... the ... is shown as a function of ... for representative values of ...
In Fig. ... the ... is shown in the form of constant-... curves given by ...
In Fig. ... we compare such results [...] with those of our ... .
Figure ... compares Eq.(...) with the exact ... for a ... and for the ...
Fig. ... and ... show the results of the ... calculations at ... and the corresponding ... .
A particularly sensitive quantity is the ... plotted in Fig. ... .
The phase diagrams plotted in the ... parts of Fig. ... correspond to ...
An example of the convergence rate of the ... for an ... is shown in Fig. 1.
The total energies as a function of ... for the ... are shown in figure ... . It can be seen that ...
To further illustrate the occurrence of ..., ... plots focusing on the ... in ... are shown in figures ... .
Our ... calculations result in the curve of Fig. ... .
Turning back to Fig. ... , we now focus on the ...
In Fig ... . Results are presented for the ... and for the ..., which were obtained from Eq. (...) by using ...
We illustrate this in Fig. ... for ..., where ...

- describing its behaviour
Concerning the ... bound, one should first note that as ... decreases, ... it is possible to construct ... .
This is the case, for example, in a ... state.
However, note that for ... reaches ... already for ... since ... .

Finally, at very large ... starts to decrease again, while at the same time, ... decreases as well.
... reaches its minimum value ... in the ... limit where ....
This type of behavior is most clearly seen for ... , while in the ... regime ... it holds only for a very limited range of ...
Upon switching on the field, this ... first decreases, but at ... it starts to increase again towards values being even higher than...
It can be seen that on the left-hand side of the plot, the ... results are very close to the ... data points, whereas on the right-hand ... the data points differ, although the deviations are only small.
Also at these larger, yet finite ... , the ... decreases and the ... region broadens substantially, while the constancy of ... still reflects the ... .
The inset shows the ... portion of the phase diagram in the ... plane, while the main plot shows the ... calculated at the critical point; all ... diverge as ...

- discussing about a figure
The most striking feature of the dispersion plot is the extraordinarily ...
One observes that the ... approximation follows rather closely the exact results for all ...
We see also that both the ... and the ... approximation are able to fit the major points of the ... results, except the exact calculations for the largest ... .
For ..., this corresponds to a ... state having ... .
Figure 1 also provides a qualitative picture of the ... dependence of ...
Comparing Figs. ... and ... , one observes that the results for ... are quite similar.
Despite the quantitative differences among the various ..., several qualitative properties are shared by all the curves: ...
... can then be reduced more efficiently for smaller ..., and therefore the ... decreases with ... .
... by comparing Figs. 1(a) and 1(b) , it can be seen that a ... algorithm converges approximately twice as fast as a simpler ... method.

5. Table

- introducing a table
The ... dependences of the ... for ... are shown in figure ... .
It can be seen in table ... that ...
... . These are shown in Table ...
The results of (i) are given in Table ..., whereas the results of (ii) and (iii) are given in Table ... .
The ... approximation assumes that the ... occurs for ... which is only valid for ... cf. Fig. ... . This means that it is assumed that in ... follow the same patterns as that of Fig. ... .

- describing/discussing about a table
As can be seen from Table ..., ... and ... for the exact calculations vary only little, indicating that our ... approach is stable against variations in the computational details.
From table ... we learn (also) that fixing ... may lead to other values of ... , but that these are also stable. According to Table ..., ...
In that figure, ... changes more slowly on changing ... than in Fig. ...

V) Discussion

1. Finding an explanation

The ... is attributed to interactions involving its ...
This is attributed to the ... as a result of ...
Moreover, the ... can also be attributed to the ... .
In the case of ..., there is a ..., hence resulting in a ... .
In fact this is easily explained. Figure ... shows ... . It can be seen that ... which ... actually belongs to the ... .
This is not simply a consequence of a ... as observed in other ... systems; in this case the ... is shortened by only ... to ... .

2. Making suppositions

This indicates that ...
The calculated ... show that ... , indicating that ... is ...
The rather rapid convergence with ... suggests that ... is not very sensitive to ...

3. Some analysis

It can also be observed that the ... increase with ...
Changing ... corresponds to moving away from ... The system will respond to this change by finding ... that leads to the smallest ...
... is a notable improvement over ... and is competitive with ... .
This is of interest for practical applications, as it will be discussed below.

4. Important remarks

A comparison of the ... is not straightforward, since ...
Moreover, ... analysis shows ...
On the other hand, the ... with the ... is quite surprising because ...
On the other hand, the ... calculations lead to markedly different values of ... .
This is, however, a problem of the ... approximation to the model and not of the ... method, as can be seen in figure 1.
It is important to stress the computational simplicity of the ... calculations, which use ...
The main advantage of the present route to ... is that ... . For example, ...

5. Comparison

Only ... provides comparable quality ... .
The ... do not provide any significant improvement.
We find that the most significant difference between the ... and ... limits affect the ... increasing the ... by approximately ...%.
From the ... analysis, only the ... demonstrate ...
In comparison with ..., ... (tend to improve) ...
Typically, ... favor ... more than ...
On the other hand, ...
Although the first method ...

6. Agreement?

This result is in good agreement with the experimental results from the group of ... showing that ...
These results agree with the observations stated in previous studies on ... regarding the ... . However, when the ... , ... occurs, and thus ...
The results agree well with previous ... calculations, although in the ... case given here, we are able to compare the difference that the ... contributions make.

7. Explanation about bad results

... . However, in the present work the focus is not on obtaining accurate ... solutions to the ... , but on demonstrating that ... calculations can provide ... values that depend only weakly on ... . We therefore consider our approach to be acceptable here.

..., our results for ... raise some doubts about whether the ... approximation is justified. However, determining both ... and ... requires more information than the ... calculations provide.

This may be due to the fact that the ... is ..., so ... with its implicit assumption of ... is an unrealistic starting point.

VI) Conclusion

Here we leave back specificities and recover generality. We point out the importance of this study and its relevance in its field. The main results and its interpretation should me mentioned, as well as possible contributions. Future studies can be pointed out.

1. Brief intro

In this paper, we examined a ... theory of ...

In this paper, we have described the implementation details of the ...

In the present paper we have first investigated the ... dependence of the ... on the ...

Following the ideas in ... from ..., we ...

We have argued that ...

We introduced ...

We have investigated the ... on ... using the ...

We have also compared ... applied to the ... formalism and also the effect of several ...

In agreement with earlier studies, we find that ...

A long standing and fundamental problem in ... has been the ... in ... . The problem is not, in fact, ... but simply requires ...

The present work introduces a ... model of the ... with the physics of ... explicitly incorporated.

A density-functional approach to ... has been applied to the ... . In this framework the basic variable is the ... .

The underlying idea, that the ..., ... is the source of ..., is elegant and easy to implement.

2. Main results

- stating the results

In the present paper we have first investigated the ... dependence of ... on the ...

We noted that ... and developed a ... for ... .

A simple general approximation to ... was then proposed which takes advantage of this ... behavior and which provides ...

Finally, using this approximation, several ground-state properties and the ... have been determined successfully as a function of ...

Rigorous results for ... were derived from

... for a test set of ... are predicted with remarkable accuracy invoking only one, universal, empirical parameter.

With a ..., a ... theory of ... interactions is obtained.

A simple general approximation to ... was then proposed which takes advantage of this ... behavior

and which provides with ... a unified description of ...
Two experimental investigations of this surface structure have been conducted, one by ... and the other by .... The first of these favoured the ..., whereas the second favoured a ... .

- agreement?
This result is consistent with the observation in Ref. ... that the ... is not ... in the limit.
Among the ..., the ... demonstrates the ... while ... shows the ... .
It was found that ... the results obtained are in excellent agreement with both experimental and other theoretical results where available.
For the ... the ... calculations reported here lead to ... that are in good agreement with experiments.
In the case of ... the agreement in the ... with that found in the published ... investigation is excellent, while there is also generally satisfactory agreement in the ... .
For ... the ... calculations reproduce the experimentally-observed preference for ..., but find two different ...
Superficially, therefore, the ... calculations fail to resolve this controversy.
In the case of ... the results are less encouraging. For ... the calculations find a ..., but the calculations show a different ... to that favoured by the ... experiment.
More quantitative evaluation of the experimental and theoretical results, however, presented in Section ... appears to marginally favour the ...
Nevertheless, these calculations all favour ..., in marked contrast to experimental studies of ...

- analysis
... achieves an accuracy comparable to that of the ...
The worst results occurred for the ... .
For ... by far the most serious problem is the clear failure of the ... calculations to produce a physically reasonable result. Specifically, these calculations fail to reveal ...
The origin of this failure is completely unknown, but extensive tests show that the result
is consistent and not simply a failure of the ... procedure. By contrast, ... calculations do all yield consistent results for a range of ... and ... broadly consistent with expectations.

On the combined test set of ... considered here, the mean signed error is ..., the mean absolute error is ..., and the RMS error is .... This accuracy is similar to that of the ..., but is based on pure, exact ... rather than a ....

- observations
For all investigated systems, ...
The observation encourages ...
Tests on ... show that ...
However, the ... calculations do show that the ...

One should not necessarily expect ...
Although the ... is highly accurate in these cases, it is not ....
Although ... data are readily available for numerous systems, these are inconvenient in general and are fundamentally problematic for ... interactions.

An analysis of these exact results shows that ... can be ...
We have supported the idea that ...

The ... model of ... achieves the goal of a ...
The ... model and ... were both easily generalized to ... . In so doing, the ... are eliminated.

The model predicts, without any empirical parameters whatsoever, ... of very good accuracy.
We applied ... successfully to ... simple models, demonstrating the high accuracy of the ... here.
These methods have been applied to ... test systems, namely, ...
The model in its present form requires the ... of each ... .

- stating the conclusions
The main conclusions of this ... can be summarized as follows...
While this conclusion appears to favour the ... proposed on the basis of the ... investigation, it is notable that the main finding of the ... study is that ...

3. Possibilities

It may be possible ...
This model ... and ... can be used to illustrate and explore problems in ... . Examples include ...
Since the ... describes the ... transition we can employ it for investigations of the ...

This ... has already been used in ..., and we hope that our ... finds fruitful applications in these areas as well.
The accuracy of the results encourages more or less straightforward applications of the present approach to related problems such as ...
It is likely that the ... will improve the accuracy of the ..., albeit at the expense of more numerical work.
In combination with a recently introduced ... model of the ..., we believe that our ... model will be the key to a robust and unified ... for all of ... .
Further theoretical investigations are being carried out on ... to explore potential applications of ... .

future works

In future work this ... will be applied to ...
The recent suggestions in Ref. ... are worth exploring, and we will do so in future work.
In future work, therefore, we will also investigate how to remove ... from the theory.
We believe that this will be rectified in future work by adding a ... term in the dispersion energy.

recommendations

For the present, we recommend ...
It should be more interesting to ...

Moreover, the possibility of generalizing the present scaling approximation to ... deserves to be investigated in detail, since it would open the way to applications in ... situations including ...
Moreover, the ... is well suited for studies of ... and of ...
In this regard a ... experimental study of the ... would be of considerable interest.

An alternative approach to this problem is the ... which has not been considered here.

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