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Electron affinities, excitation energies and ionization potentials of the transition metals (I) Sc and Ti

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Abstract. The electron affinities of the Sc and Ti atoms have been obtained by configuration interaction calculations. Energy convergence with respect to the systematic expansion of both the one-electron basis set and the configuration space was investigated for valence electrons, and the inclusion of correlation contributions from core electrons and relativistic effects gave the electron affinities of 0.181 eV and 0.163 eV for Sc and Ti, respectively. These are in excellent agreement with the observed values of 0.189 ± 0.020 eV and 0.080 eV. The same approach was applied for the first excited states and positive ions of both atoms. Excellent agreement with the experimental results was also obtained for these states.

Key words: Electron affinity – Excitation energy – Ionization potential – Energy convergence – Transition metal atoms

1 Introduction

To obtain an accurate electron affinity (EA), one has to calculate the total energies for both the neutral and negatively ionized systems with equivalent accuracy. It is necessary to compute an accurate differential correlation effect between two systems possessing different numbers of electrons. This is one of the fundamental difficulties in computational chemistry. In this work, the EAs of Sc and Ti were investigated. The electronic structures of transition metals are, in general, complicated because of the strong interaction between the $3d$ and $4s$ shells, which has a strong dependence on the occupation of the $3d$ shell. When an extra electron attaches to a transition metal atom, it usually occupies the $3d$ orbital, as is the case with Ti. Therefore, in order to determine accurate EAs for such systems, one must also account for the

differential correlation effect between the two systems having different numbers of $3d$ electrons. In Sc, on the other hand, the extra electron occupies the p-orbital, as with the alkaline-earth atoms. The ground state of Sc$^-$ has been established experimentally as $3d4s^24p$, and subsequent calculations by Jeung [1] and Bauschilcher et al. [2] have determined the term as $^1D^o$.

Extensive calculations have been performed by Bauschlicher et al. [2] and Froese Fischer and Brage [3]. Bauschlicher et al. have calculated the EA of Sc and Ti by second-order configuration interaction (SOCI) using an extended GTF set. They considered only the valence correlation. To avoid the effects of the correlation contribution from the $3s$ and $3p$ electrons, they computed EAs relative to an excited state with the same number of d-electrons. For Ti, they used the $3d^34s^1$ excited state as the reference and adjusted the value to the ground state of the atom using the known experimental atomic separation. They reported EAs for Sc and Ti in excellent agreement with experimental values without considering relativistic effects. For Sc, Froese Fischer and Brage [3] have performed multi-configuration Hartree-Fock (MCHF) calculation with an active set of 3-5d, 4-6s, 4-6p, 4-5f and $5g$ orbitals expanded in numerical orbitals to account for the valence correlation and obtained an EA of 0.226 eV. They restricted the size of the MCHF wave functions by deleting unimportant configuration state functions and included the polarization potential for the $3p^6$ ^1S core. Furthermore, they considered relativistic effects. These effects reduced the EA by 43 meV, and they finally obtained a value of 0.183 eV.

It is clear that an accurate EA of transition metal atoms cannot be obtained by considering only the correlation effects of the $3d$, $4s$ and $4p$ valence electrons, and that both the correlation contributions from $3s$ and $3p$ electrons and relativistic effect must also be taken into account. Previous theoretical studies, however, have not include these effects sufficiently. Thus, the purpose of the present work is to obtain accurate EAs for Sc and Ti by considering the correlation effects of $3s$ and $3p$ electrons explicitly and including the relativistic effect. The contributions considered in the present work are classified as

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follows, together with the definition of the terminology used in this paper.

1. Valence correlation: is defined as the correlation among the $3d$ and $4s$ electrons. For Sc$^-$, the $4p$ electron is also included in the valence shell. The valence correlation is usually the main contribution to the differential correlation effect.
2. Core-valence and core correlation: consider the $3s$ and $3p$ electrons as core electrons. The correlation effects among the $3s$, $3p$ and $3d$ electrons are expected to be rather large. Therefore, these correlations cannot be ignored when accounting for the differential correlation effects between two systems possessing a different number of $3d$ electrons.
3. Relativistic effects: it is known that relativistic effects stabilize $4s$ electrons and destabilize $3d$ electrons. Thus, these effects contribute to the energies of the transitions that cause changes in the occupations of the $3d$ and $4s$ shells.

In the study of valence correlation, energy convergence with respect to both the one-electron basis set and the configuration space was investigated. A series of SDCI calculations was performed with increasing an angular momentum (l) of the basis functions to obtain the remainder of the higher l-functions. Multi-reference CI (MRCI) calculations were then repeated with increasing reference configuration, and the CI energies were plotted against the weight of the reference configurations in the MRCI wave function to investigate the convergence in the configuration base. The same approach was used, and yielded extremely accurate EAs for small systems [4, 5].

For correlation contributions from the core electrons, the ideal approach is to investigate the convergence of the basis set and the configuration space by considering the valence and core electrons simultaneously. However, the additional eight electrons make this approach impossible due to limitation of computational resources. Instead, a simple multi-reference single and double excitation CI (MRSDCI) calculation was carried out to account for the core electron contributions, including the important valence excitations in the reference space. Assuming an additivity of valence and core correlation effects, we evaluated the EAs for both Sc and Ti. Finally, Dirac-Fock calculation were carried out to investigate the relativistic contributions to the EAs.

The same approach was applied to the first excited states and the positive ionic states of both atoms. Martin and Hay [6] investigated relativistic effects using the numerical HF calculations and the approximate scheme of Cowan and Griffin for these states. They showed that relativistic corrections are surprisingly large even for the first transition metals. A systematic study on the excited states of transition metal atoms was performed by Bauschlicher et al. [7]. They performed a SCF/CI calculation using a large basis set and yielded a good agreement with the experimental separation for the lowest states of $3d^n4s^2 - 3d^{n+1}4s$. Inclusion of f^- functions gave 0.1 eV effect and the $3s3p$ correlations yielded another 0.26–27 eV for the separations.

In the present study, we investigated the l-convergence, convergence to the full CI limit, and contributions from the core and relativistic effects for these states. These results would be expected to provide good reference points for molecular calculations.

In the next section, we describe the calculational procedure. The results and discussion are given in Sect. 3 followed by our concluding remarks.

2 Method of calculation

The following states were considered in the present work:

Sc$^+$	$3d4s$ (^3D),	$4s^2$(^1S)
Sc	$3d4s^2$ (^2D),	$3d^24s$ (^4F)
Sc$^-$	$3d4s^24p$ ($^{1,3}D^o$)	
Ti$^+$	$3d4s^2$ (^2D),	$3d^24s$ (^4F)
Ti	$3d^24s^2$ (^3F)	$3d^34s$ (^5F)
Ti$^-$	$3d^34s^2$ (^5F).	

2.1 Basis set

We used a Slater-type function (STF) basis set, which consists of the $1\text{-}2s$ and $2p$ STFs of Clementi and Roetti [8] augmented by even-tempered sequences of $3s$, $3p$, $3d$, $4f$, $5g$ and $6h$ STFs. The ratios of the sequences were $\sqrt{2}$. The exponents of the first $3s$ and $3p$ STFs were the same as those of the outermost $2s$ and $2p$ STFs, respectively. For the first $3d$ STF, we also used the same exponents as the outermost $2p$ STF. In order to used the sizes of the s–d sequences, we repeated MRSD CI calculations using s–d basis functions. In these calculations, we considered only the valence excitations from a reference space which consists of the HF configuration and those generated by the excitation $4s^2 \rightarrow 4p^2$ and $3d^2 \rightarrow 4d^2$. Hereafter, we call this a minimal reference space. The number of the basis functions was increased until the energy lowering of an additional STF was less than 1.0×10^{-5} a.u.

The orbital exponents of the $4f$, $5g$ and $6h$ STFs were chosen so that their extents were the same as those of the $3d$ STFs.

The basis set was determined individually for each state by using the above procedure. The sizes of the basis sets thus determined are $11\text{-}15s$ $10\text{-}14p$ $7\text{-}11d$ $7\text{-}11f$ $7\text{-}11g$ $7\text{-}11h$, in which we used large sets such as $15s13p10d10f10g10h$ and $14s14p11d11f11g11h$ for Sc$^-$ and Ti$^-$, respectively. These STF basis sets reproduce the HF limits in 0.0004 a.u. for all states.

All calculations were performed on an IBM/RS6000 system using the ATOMCI [9, 10] and GRASP2 [11] programs for CI and Dirac-Fock calculations, respectively.

2.2 Valence correlation

We investigated the l-convergence by a series of MRSDCI calculations with the minimal reference space, using the spd, $spdf$, $spdfg$ and $spdfgh$ sets. In each step of the calculations, natural orbitals (NOs) were generated for use in the subsequent steps. The spd NOs were generated from CI with spd STFs, and f NOs from CI with spd NOs $+ f$ STFs, and so on. In order to reduce the size of the calculations, we truncated those NOs whose occupation numbers were less than 1.0×10^{-6} at each step. The effects of truncating NOs from the external space were studied by comparing two sets of CI energies, one calculated with a full basis set and the other with a truncated set for each l.

We repeated the MRSDCI calculations with increasing reference configurations which were chosen for the largest weight in the previous CI wave functions with the minimal reference space. The multi-reference analogue of Davidson's correction [12] (denoted

as +Q) was also computed. The calculated CI and CI + Q energies are plotted against the weight of reference space (*w*), and the full CI limit is then obtained by extrapolating the curves to $w = 1$ where the CI and CI + Q energies coincide with each other.

2.3 Core-valence and core correlation

To estimate the core-valence and core-correlation effect we performed a restricted MRSDCI calculation, in which the excitations were limited to simultaneous excitations of the core and valence electrons or double excitations of the core electrons from a reference space. Hereafter, these two types of CIs will be referred to as CV-CI and C-CI. Single excitations from the core electrons were considered in CV-CI. First, in order to prepare compact and appropriate external orbitals to express the core-valence and core correlations, we carried out these two types of CI calculations with the minimal reference functions. In these calculations, we generated and selected the external NOs stepwise in the same manner as the valence CI. We also investigated the *l*-convergence of core-valence and core correlations. Here, the core-valence and core-correlation energies are defined as the difference between the CI energies and the reference energies. For Ti, the stability of the core-valence and core-correlation energies was assessed by increasing the reference configurations, which were selected only from the valence CI wave functions.

2.4 Relativistic effect

The relativistic effects were studied by comparing the HF and Dirac-Fock [11] energies. For Sc⁻, we employed an MCSCF calculation with two configurations including $3d4s^24p$ and $3d4p^3$. In the relativistic calculations, we calculated all possible *jj* terms and took a weighted average of the resulting values to obtain the HF energies of the *LS* terms.

3 Results and discussion

The excitation energies, EAs and ionization potentials (IPs) obtained at each calculational level are summarized in Tables 1 and 2 together with the total energies of the ground state. We also list the previous theoretical results and the available experimental results for comparison.

In the valence CI, errors due to the truncation of the NOs are less than 1.0×10^{-4} a.u. for all states, and the effects on the relative energies are less than 5.0×10^{-5} a.u. In Fig. 1, we plot the contributions to the correlation energies from respective *l*-values in a log-log scale. Clearly, all of the convergence patterns are on straight lines. Assuming this linear form, we can estimate the remainders from higher angular momenta than *h*. The contributions from the remainder to the total energies are around 1.0×10^{-4} a.u., thus having only a small effect on the relative energies. The CI and CI + Q energies are plotted against the weight of the reference space *w* for the neutral ground state and negatively ionized states as shown in Figs. 2 and 3 for Sc and Ti, respectively. The valence-full CI limits were then ob-

Table 1. The excitation energy, electron affinities (EAs), and ionization potentials (IPs) (in eV) of the Sc atom. For the ²D state, the total energy (+ 759 a.u.) given

	Sc		Sc⁻		Sc⁺	
	^2D $3d4s^2$	^4F $3d^24s$	$^1D^o$	$^3D^o$ $3d4s^24p$	^3D $3d4s$	^1S $4s^2$
MCSCF	−0.76357	1.560	−0.666	−0.804	6.113	7.379
Valence						
MRSDCI	−0.77926	1.613	0.252	0.093	6.403	7.682
Full-CI	−0.77926	1.613	0.253	0.093	6.400	7.679
Truncated NOs[a]	−0.77930	1.613	0.253	0.094	6.413	7.680
Higher *l* STF s[a]	−0.77935	1.613	0.253	0.094	6.413	7.680
Core-valence and Core						
CV-CI[a]	−0.86961	0.889	0.210	0.074	6.510	8.806
Truncated NOs[a]	−0.86970	0.890	0.210	0.074	6.509	8.808
Higher *l* STFs[a]	−0.87416	0.922	0.208	0.074	6.509	8.851
C-CI[a]	−1.12948	1.334	0.230	0.079	6.532	8.246
Truncated NOs[a]	−1.12975	1.335	0.235	0.079	6.533	8.249
Higher *l* STFs[a]	−1.13698	1.330	0.234	0.079	6.535	8.258
Relativistic effects[a]						
	−4.78001	1.464	0.181	0.050	6.568	8.066
Other theoretical calculations and experiments						
CI		1.66[b]	0.195[c]	0.011[c]		
MCHF[d]			0.2257	0.0567		
MCHF + core + RS[e]			0.1831	0.0302		
Observed		1.440[f]	0.189[g]	0.042[g]	6.561[f]	8.016[f]

[a] The estimated contribution is added to the energy obtained in the previous step
[b] MCSCF/CI calculation by Bauschlicher et al. [7]
[c] SOCI calculation by Bauschlicher et al. [2]
[d] MCHF calculation considering only valence correlation by Froese Fischer and Brage [3]
[e] MCHF calculation including the core polarization and the relativistic effects by Froese Fischer and Brage [3]
[f] Baschkin and Storner [15]
[g] Feigerle et al. [14]

Table 2. The excitation energy, EA and IPs (in eV) of the Ti atom. For the Ti ^3F state, the total energies ($+848$ a.u.) are given

| | Ti | | Ti$^-$ | Ti$^+$ | | | |
| | ^3F $3d^24s^2$ | ^5F $3d^34s$ | ^4F $3d^34s^2$ | ^4F $3d^24s$ | ^2D | | |
					$3d^24s$	$3d^3$	$3d4s^2$
MCSCF	−0.43435	0.810	−0.633	6.290			9.436
Valence							
MRSDCI	−0.46468	0.923	−0.036	6.678	8.128	9.212	9.904
Full-CI	−0.46473	0.925	−0.034	6.680	8.129	9.214	9.905
Truncated NOs[a]	−0.46478	0.925	−0.033	6.680	8.128	9.213	9.906
Higher l STFs[a]	−0.46496	0.925	−0.032	6.683	8.124	9.203	9.907
Core-valence and Core							
CV-CI[a]	−0.61196	0.284	0.557	6.809	8.253	7.796	10.497
Truncated NOs[a]	−0.61212	0.285	0.557	6.809	8.253	7.796	10.498
Higher l STFs[a]	−0.61613	0.254	0.584	6.808	8.229	7.807	10.487
C-CI[a]	−0.85466	0.562	0.338	6.816	7.974	7.986	9.693
Truncated NOs[a]	−0.85481	0.562	0.338	6.817	7.973	7.986	9.692
Higher l STFs[a]	−0.86282	0.555	0.344	6.816	7.973	7.975	9.703
Relativistic effects[a]							
	−5.31204	0.718	0.163	6.869	7.993	8.175	9.471
Other theoretical calculations and experiments							
CI		0.94[b]	0.002[c]				
Observed		0.834[d]	0.080[e]	6.821[d]	7.903[d]	8.405[d]	9.963[d]

[a] The estimated contribution is added to the energy obtained in the previous step
[b] MCSCF/CI calculation by Bauschlicher et al. [7]
[c] SOCI calculation by Bauschlicher et al. [2]
[d] Baschkin and Stoner [15]
[e] Feigerle et al. [16]

tained by extrapolating the curves to $w = 1$. The same investigations were carried out for the other states.

In the CV-CI and C-CI, the errors due to the truncation of NOs and higher l-orbitals are larger by one order of magnitude than those in the valence case, but the effects on the relative energies are still small. The stability of the calculated core-valence and core-correlation energies was investigated by increasing the reference configurations. We plot the core-valence and core-correlation energies against the weight of the reference space w in Figs 4 and 5, respectively. These correlation energies are stable within 0.001 a.u. at the CI calculation with the largest set of the reference configurations. Thus we give those core-valence and core-correlation energies in Tables 1 and 2.

As shown in Tables 1 and 2, the relativistic effects in each electronic state are different from one another. The large relativistic corrections occur for the transitions where the occupation of $3d$ electron changes.

3.1 Electron affinity

For Sc, we obtained EAs of 0.253 and 0.094 eV for $^1D^o$ and $^3D^o$, respectively including the remainder of the higher l-contributions and the effect of the discarded NOs at the valence CI level. These values are slightly larger than the values of 0.226 and 0.057 eV obtained by Froese Fischer and Brage [3]. On the other hand, Bauschlicher et al. [2] obtained EAs of 0.195 and 0.011 eV, which are in excellent agreement with experimental values. This agreement comes from the poor

description of Sc$^-$ as compared to Sc. They included only the $3d$, $4s$ and $4p$ orbitals in the active space of SOCI. To reach the same accuracy with Sc, we need to add $4f$ and $4d$ to represent the reference CSFs for Sc$^-$. The present study shows that the inclusion of the core correlation decreases the EAs by 0.019 and 0.015 eV for $^1D^o$ and $^3D^o$, respectively. The same tendency can be seen in the calculation by Froese Fischer and Brage, although the treatments of the core correlation are different from one another. In their calculation, the core-polarization correction reduces the EAs of $^1D^o$ and $^3D^o$ by 0.034 and 0.014 eV, respectively. The relativistic correction in our study decreased EAs by 0.053 and 0.029 eV for $^1D^o$ and $^3D^o$, respectively. These corrections are significantly larger than the previous theoretical values of ~ 0.008 eV [3, 13]. We performed a MC Dirac-Fock calculation including $3d4s^24p$ and $3d4p^3$ in the reference space, since a single configuration SCF gives a continnum state $3d4s^2\epsilon p$. The final EAs of 0.181 and 0.050 eV for the $^1D^o$ and $^3D^o$ states are in good agreement with the observed value.

For Ti, a negative EA of -0.032 eV was obtained at the valence CI level. Bauschlicher et al. have given an EA of 0.002 eV by calculating the energy of Ti$^-$ relative to Ti(^5F), which has the same occupation in the $3d$ shell, and adding the experimental excitation energy. Application of the same procedure to the present results provides an EA of 0.059 eV, which is in good agreement with the experimental value of 0.080 eV. Indeed, the contribution of the differential correlation effect from the core electrons can be avoided by using this procedure. However, Bauschlicher et al. have underestimated
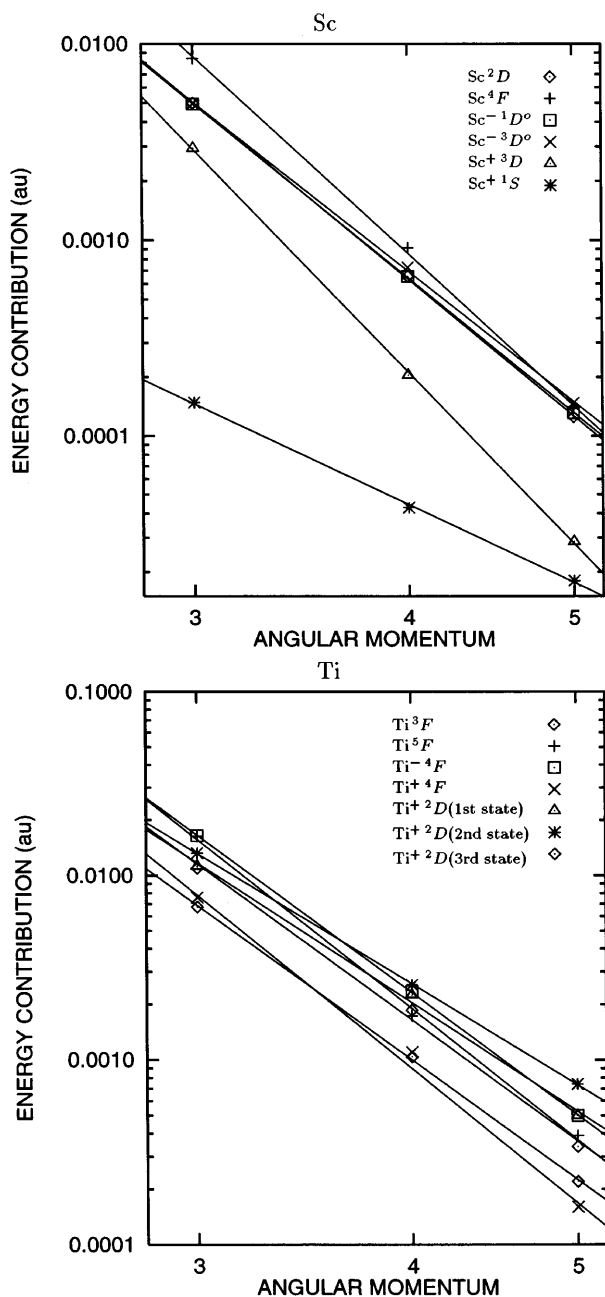
Sc

Sc ^2D	◇
Sc ^4F	+
Sc$^-$ $^1D^o$	⊡
Sc$^-$ $^3D^o$	×
Sc$^+$ ^3D	△
Sc$^+$ ^1S	✳

Ti

Ti ^3F	◇
Ti ^5F	+
Ti$^-$ ^4F	⊡
Ti$^+$ ^4F	×
Ti$^+$ ^2D(1st state)	△
Ti$^+$ ^2D(2nd state)	✳
Ti$^+$ ^2D(3rd state)	◇

Fig. 1. Contributions to the correlation energy from different l

Fig. 2. Convergence patterns of MRSDCI and MRSDCI + Q energies as a function of the weight of the reference space for Sc and Sc$^-$ $^1D^o$

Fig. 3. Convergence patterns of MRSDCI and MRSDCI + Q energies as a function of the weight of the reference space for Ti and Ti$^-$

the EA for Ti. The contribution from the core is larger by one order of magnitude than that for Sc and yielded a positive EA of 0.344 eV. This suggests that the core-correlation effect is essential in accounting for the differential correlation between Ti and Ti$^-$. The relativistic correction decreases the EA by 0.181 eV. This is because the extra electron is added to the destabilized $3d$ orbital. The resultant EA of 0.163 eV is larger than the experimental EA by 0.083 eV. In the present calculations, we could not consider the coupling among valence correlations, core correlations, and relativistic effects. In order to reproduce such a small EA, it may be necessary to consider this coupling.
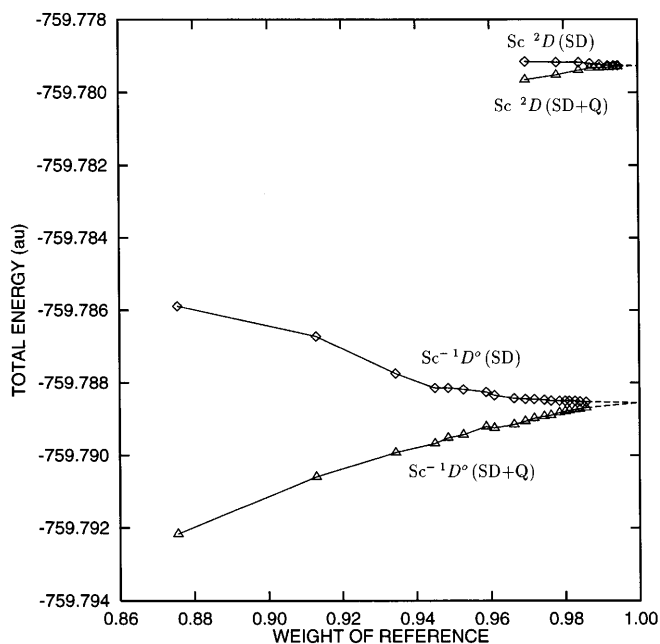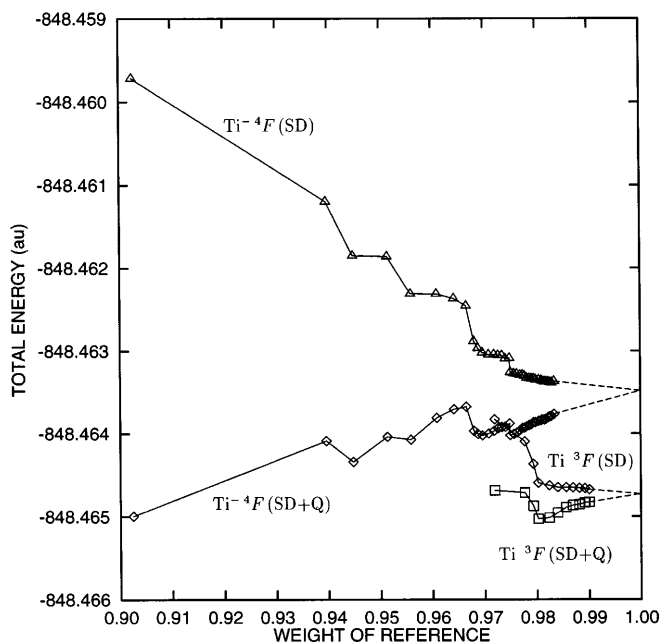
3.2 Excitation energies

The ^4F excited state of Sc has a $3d^24s$ configuration, which has a different $3d$ occupation from the ground state. The valence-full CI limit gave 1.613 eV compared with the experimental value of 1.440 eV. The core effect decreased the excitation energy by 0.238 eV, and the relativistic effect increased it by 0.134 eV. Finally, we
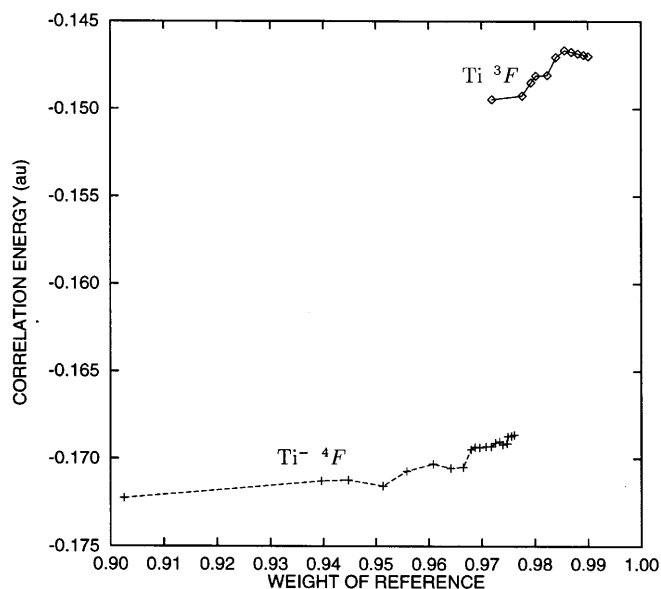
Fig. 4. The core-valence correlation energies as a function of the weight of the reference space in the valence MRSDCI wave functions of Ti and Ti$^-$

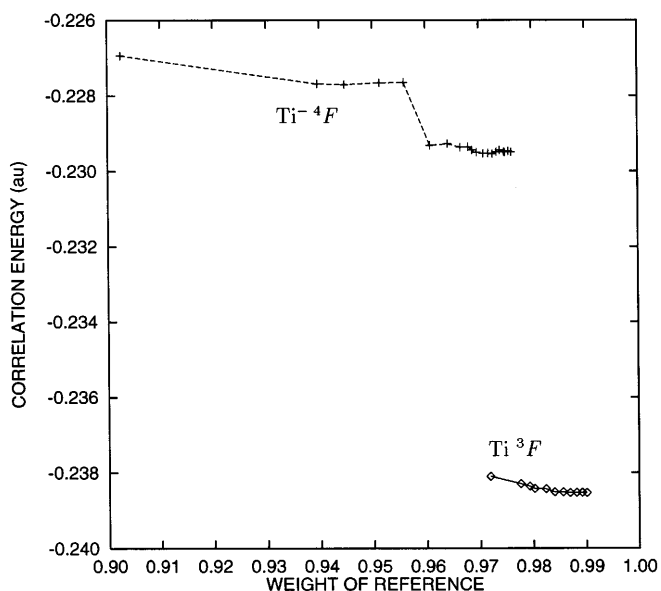**Fig. 5.** The core correlation energies as a function of the weight of the reference space in the valence MRSDCI wave functions of Ti and Ti$^-$

3.3 Ionization potentials

The valence CI gave good IPs for the $4s$ electron both for Sc and Ti. We obtained 6.413 and 6.683 eV for ^3D and ^4F, respectively. These values are in agreement with the experimental values of 6.561 and 6.821 eV. The core contributions and the relativistic effect reduce the small discrepancy and yield final results of 6.568 and 6.869 eV, which are within 0.007 and 0.048 eV of the experimental values, respectively.

On the other hand, the ionization of the $3d$ electron changes the situation dramatically. For the $4s^2$ ^1S ionized state of Sc$^+$, the valence CI gave an IP of 7.680 eV, which is 0.336 eV smaller than the observed value. The inclusion of the core and relativistic effects reduced this discrepancy, giving a value in almost complete agreement with the experimental results.

The $3d4s^2$ ^2D ionized state of Ti$^+$ was obtained as the third solution of the valence CI calculations for the ^2D states. The lowest solution is $3d^24s$ and the second is $3d^3$. The valence CI gave IPs of 8.124, 9.203 and 9.907 eV for $3d^24s$, $3d^3$ and $3d4s^2$, respectively, which differs from the observed values by 0.221 eV, 0.798 eV and 0.056 eV. By including the core and relativistic effects, we could obtain the lowerst ^2D ionized state with the same accuracy as the other states, but we could not achieve a comparable accuracy for the higher two ^2D ionized states, $3d^3$ and $3d4s^2$. The core-valence and core-correlation energies estimated here may not be as reliable as those for the other states. The lowest three solutions of the valence CI have the main configurations of $3d^24s$, $3d^3$ and $3d4s^2$. However, these configurations mix strongly in CV-CI and C-CI, and the characters of the wave functions change noticeably. This means that the coupling between the valence and core correlations is significantly large, and the assumption of additivity for these correlation effects becomes inadequate. The Dirac-Fock approximations may also not give a reliable estimation of the relativistic effects for these states. Moreover, the coupling among the valence correlations, core correlations and relativistic effects is essential, although this coupling could not be considered in the present work.

4 Summary

Systematic MRCI calculations were performed on the Sc and Ti atoms. Convergence for both the basis functions and the configuration basis was investigated at the valence CI level. Core-valence and core-correlation energies and relativistic effects were estimated separately. Assuming the additivity of these contributions, the excitation energies, EAs, and IPs were calculated in excellent agreement with the observed values, except for the ionization of the $3d$ electron of Ti where could not obtain a reliable IP. In order to obtain more reliable results, the coupling among the valence correlations, core correlations and relativistic effects must be considered. The values reported in this paper will provide good reference points for molecular calculations.

obtained 1.464 eV for the excitation energy, which is in excellent agreement with the experimental value. Bauschlicher et al. [7] have obtained a slightly larger excitation energy of 1.66 eV by the MCSCF/CI method using three f functions.

The ^5F excited state of Ti also arises from the excitation of $4s$ to $3d$ and shows the same tendency with ^4F of Sc. The valence CI limit yielded 0.925 eV, the core effect decreased the excitation energy by 0.370 eV, and the relativistic effect increased it by 0.164 eV. The final result is 0.718 eV, which is 0.116 eV smaller than the observed value.

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