CI Calculations of the Ground State Ionization Potential and Electron Affinity of Aluminum

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Nonrelativistic configuration interaction study for Al^+, Al and Al^- are presented, included calculations of ionization potential and electron affinity of the $^2P^o$ ground state of Al. CI calculations up to double, triple and quadrupole excitations for Al^+, Al and Al^-, respectively, where neon fixed core is considered. Appropriate Slater type basis functions were developed suitable to recover both of core-valence and core–core correlation effect. The relativistic effect on both ionization potential and electron affinity are taken into account at the relativistic Hartree–Fock level. The calculated electron affinity is 432.811 meV which is in excellent agreement with experimental value of Sheer et al. 432.83(5) meV, whereas the calculated ionization potential is 5985.764 meV, the latter is in perfect agreement with experimental value of 5985.768 meV.

1. Introduction

During the past years, many calculations of electron affinity (EA) were carried out on the ground state $^2P^o$ of Al with respect to ground state ^3P of Al, these calculations were started in 1992 with Arnau et al. [1] where they applied configuration interaction (CI) with pseudopotentials and obtained an EA of 450 meV.

Dunning and co-workers [2, 3] have developed families of Gaussian basis sets optimized for correlated calculations on the valence electrons of atoms and molecules, these basis sets later used to calculate electron affinity with multireference single and double excitation configuration interaction (MRSD-CI) with the augmented correlation consistent polarized valence basis set (aug-cc-pvDZ) and reported an EA of 437 meV [4]. Eliav et al. applied relativistic coupled-cluster (RCC) method in a large four-component Gaussian-spinor basis to calculate electron affinities as well as ionization potential (IP) of group-13 elements including Al and reported an EA of 427 meV and IP of 5991 meV [5]. In the same year, multiconfiguration Dirac–Fock (MCDF) method due to Wijesundera [6] were used through out to obtain an EA of 433 meV. Benchmark *ab initio* and density functional calculations by de Oliveira et al. [7] has yielded an EA, which agrees with the last experimental value of Scheer et al. [8]. The important feature of de Oliveira calculations is the inclusion of inner-shell correlation (core–valence interaction) which lead to crucial contribution to EA.

The present work introduces a suitably developed one-electron basis set of the Slater type orbital (STO) to treat both core–valence and core–core correlation effects. These basis set are equivalent to Gaussian basis set of

Dunning and co-workers (correlation consistent polarized core–valence cc-pCVXZ) [9]. These basis set are used to calculate accurate electron affinity and ionization potential of the ground state of aluminum in the frame work of nonrelativistic CI method.

CI calculations up to triple and quadrupole excitations are limited to valence correlation calculation where the negative ion Al and the neutral atom Al are treated as four- and three-electron system, respectively. The relativistic correction is added at the Dirac–Fock level by making relativistic Hartree–Fock calculations on the related levels ^1S, $^2P_{1/2}$, and ^3P. In Sect. 2, we describe the CI theory employed to calculate ionization potential and electron affinity and where we briefly review the construction of the CI wave function. The orbital basis set used are taken up in Sect. 3. In Sect. 4, the approach of the approximate full configuration interaction (FCI) in the frame work of a priori selected configuration interaction (SCI) with its corresponding truncation energy error [10] and CI by parts CIBP [11] are presented. Results and discussion is presented in Sect. 5 and finally conclusions are drawn in Sect. 6.

2. CI theory

The matrix form of the Schrödinger equation is

$$\boldsymbol{H}\boldsymbol{C}_\mu = E_\mu^{\text{FCI}}\boldsymbol{C}_\mu, \tag{1}$$

where E_μ^{FCI} is the full CI energy which is an upper bound energy of the system under consideration, $\boldsymbol{C}_\mu$ is column vector of the CI coefficients, and $\boldsymbol{H}$ is the matrix element representation in terms of the Slater determinants or N-electron symmetry eigenfunctions constructed from given orbital basis.

In CI nomenclature, Eq. (1) is called full CI (FCI) equation [12].

The exact eigenvalue E_μ of the Schrödinger equation can be expressed as

$$E_\mu = E_\mu^{\text{FCI}} + \Delta E_\mu^{\text{OBI}}, \tag{2}$$

where $\Delta E_\mu^{\text{OBI}}$ is the basis set incompleteness error [13].

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In CI approach the many electron wave function is expanded as linear combination of configuration state functions F_{gK} [14]:

$$\Psi = \sum_{K=1}^{K_x} \sum_{g=1}^{g_K} F_{gK} C_{gK}. \tag{3}$$

The configuration state function F_{gK} are obtained as successively orthogonalized symmetric projections of Slater determinants, they may be expressed as linear combination of n_k Slater determinants D_{iK}:

$$F_{gK} = O(L^2, S^2) \sum_{i=1}^{g} D_{iK} b_i^g = \sum_{i=1}^{n_K} D_{iK} c_i^g, \tag{4}$$

where $O(L^2, S^2)$ are idempotent projection operators for L^2 and S^2. K and g labels for configuration and degenerate element, respectively.

Triply and higher excited configurations are classified into disconnected and connected ones. Disconnected configurations are those that can be expressed as products of combinations of lower excited ones, whereas connected configurations are all others [10].

In general, the set of all excited configurations, F_{gK} are divided into classes and in turn all configurations differing just in the labels of the virtual orbital radial functions are called subclass, where the coefficients b_i^g and c_i^g in Eq. (4) are the same for different configurations within a given subclass.

3. Basis set construction

In our calculations, the radial part R_{il} of the orbital is expressed as linear combination of normalized Slater type orbital STOs S_{jl}:

$$R_{il} = \sum_j S_{jl} a_{jli}, \tag{5}$$

where

$$S_{jl} = N_{jl} r^{(n_j - 1)} \exp(-Z_{jl} r), \tag{6}$$

$$N_{jl} = (2Z_{jl})^{(n_j + 1/2)} [(2n_j)!]^{-1/2}. \tag{7}$$

The representation of orbitals in terms of STOs for valence CI calculations of Al and Al$^+$ are developed from initial STOs of the Hartree–Fock [15] quality of $9s$ and $8P$, and an additional reoptimized functions of $3d$ and $2f$ were considered to describe the diffuse charge distribution of Al$^-$. Thereafter, the correlation orbital space wave function is expanded by inclusion all singles and doubles excitations outside the neon fixed core up to orbital harmonic $l = 20$, leading to 121, 168 and 186 energy optimized STOs for ^1S, $^2P^o$ and ^3P states respectively, where it is important to maintain the initial $9s$ and $8P$ fixed during the optimization process. Later the resulting final basis set are used to make the valence correlation full CI calculations for Al and Al$^-$ as will be discussed in the next section.

For valence–core and core–core CI calculations, the same initial STOs are used as that for valence calculations except that all pure single and double excited configurations outside neon fixed core are excluded from the configuration list, thus only pure single and double excited configurations coming from the core as well those configurations coming from mixed double excitations from neon core and valence electrons outside the core are included in the CI expansion.

In our work both core–valence (CV) configuration interaction calculation and core–core (CC) configuration interaction calculation are done together and we denoted them by CVCC, work is in progress to separate both components.

4. CI techniques

Two CI techniques were performed throughout this work, the first one is the priori SCI to approximate full CI which where done by the program AUTOCL [14]. The new version of the mentioned program consists more compact and efficient energy selection thresholds for selection of subclasses and configurations.

The selection of disconnected configurations are based on the Brown formula [16]:

$$\Delta E_K = (E - H_{KK}) B^2{}_K / \left(1 - B^2{}_K\right), \tag{8}$$

where E is any pertinent energy, $H_K K$ is the diagonal matrix element which can be well approximated by the expectation value of any determinant belonging to the configuration K, and B_K is an approximation to the configuration coefficient associated with triple and higher excited disconnected configurations [10]. The selection of q-excited connected configurations are based on modified Brown formula [17]:

$$\Delta E_K^{\mathrm{pgy}} = (E - H_{KK}) \prod_{i=1}^{q} n_{K_i}, \tag{9}$$

where n_{K_i} are the occupation numbers of the natural orbital which are implemented to approximate the correlation orbitals.

All triply and higher disconnected subclasses with enrgy contributions lesser than an energy threshold $T_{\mathrm{subc}}^{\mathrm{egy}}$ are discarded and accumulated into the total truncation energy error ΔE^{egy}, while the triply and higher connected subclasses with an energy contribution lesser than an energy threshold $T_{\mathrm{subc}}^{\mathrm{pgy}}$ are discarded and accumulated into the total truncation energy error ΔE^{pgy} such that

$$\Delta E^{\mathrm{egy}} = \sum_{\mathrm{deleted\ subc}} \Delta E_{\mathrm{subc}}^{\mathrm{dis}} \tag{10}$$

and

$$\Delta E^{\mathrm{pgy}} = \sum_{\mathrm{deleted\ subc}} \Delta E_{\mathrm{subc}}^{\mathrm{con}}, \tag{11}$$

where

$$\Delta E_{\mathrm{subc}}^{\mathrm{dis}} = \sum_K \Delta E_K \tag{12}$$

and

$$\Delta E_{\mathrm{subc}}^{\mathrm{con}} = \sum_K \Delta E_K^{\mathrm{pgy}}. \tag{13}$$

Selection of subclasses reduce the FCI size of energy E^{FCI} into a condensed space (model space) M of energy E_M

and truncation energy errors of ΔE_M^{egy} and ΔE_M^{pgy} associated with that model space

$$E^{\text{FCI}} = E_M + \Delta E_M^{\text{egy}} + \Delta E_M^{\text{pgy}}. \qquad (14)$$

Because the size of model space is still too high to solve its corresponding eigenvalue problem, therefore another selection process is made on individual configurations. The program ATMOL is used to perform another selection with different values of energy and pseudo energy selection thresholds for each excitation of disconnected and connected configurations respectively to reduce the size of the model space to more condensed space S:

$$E_M = E_S + \Delta E_S^{\text{egy}} + \Delta E_S^{\text{pgy}}, \qquad (15)$$

where the meanings of ΔE_S^{egy} and
ΔE_S^{pgy} are identical as those in Eq. (14), except that the sums in Eqs. (10) and (11) are run over deleted configuration rather than subclasses.

The next step taken by the program ATMOL is the CI by part CIBP, where the S-space is partitioned into several subspaces $S_0, S_1, S_2, \ldots, S_r$ of dimensions $d_0, d_1, d_2, \ldots, d_r$, respectively, where S_0 is the reference space in which all CI coefficients are always variational, and all other subspaces $S_i, i = 1, 2, \ldots, r$ will be taken up variationally one after the other [18].

The final eigenvalue will satisfy

$$E_S = E_{\text{CIBP}} + \Delta E_{\text{CIBP}}, \qquad (16)$$

where ΔE_{CIBP} is the error due to CIBP method which can be determined through sensitivity analysis, where ΔE_{CIBP} is necessarily a positive quantity. In order to make ΔE_{CIBP} rather small, the energy corresponding to $S_0 + S_1$ must be as close as possible to E_{CIBP}, thus pushing up values of $d_0 + d_1$ that require solving the eigenvalue problem outside RAM. After S_1 is processed, however, the remaining subspaces S_i (i greater than 1) are (automatically) chosen so that all matrix elements in $d_0 + (i - 1) + d_i$ fit in RAM [19].

5. Results and discussion

In this work, nonrelativistic CI calculations of ionization potential and electron affinity are divided into two components, the first one is the valence correlation component and the second one is CVCC correlation component. The first component included configuration interaction calculations of IP and EA at neon fixed core approximation, where only two, three and four electrons correlation for $\text{Al}^{+1}S$, Al^2P^o and $\text{Al}^{-\ 3}P$ states respectively are considered. In this stage of calculation, excitations up to double, triple and quadrupole for ^1S, $^2P^o$ and ^3P states, respectively.

Table I shows angular momentum–energy convergence at singles and doubles excitations level (SD) up to harmonic $l = 20$ for ^1S, $^2P^o$ and ^3P states for valence correlation CI calculations. The pattern of ^3P state shows the slowest energy convergence with respect to both ^1S and $^2P^o$ states, and the ^1S state show the fast energy convergence pattern.

TABLE I

Angular momentum-energy convergence of Al^+ ^1S, Al^- $^2P^o$ and Al^- ^3P states for CISD valence calculations. Total energies E (in Ha) and energy-convergence ΔE (in μHa).

$l_{\max}$	E (Al^+ ^1S)	ΔE	E (Al^- $^2P^o$)	ΔE	E (Al^- ^3P)	ΔE
1	-241.7133874116		-241.9076962793		-241.9104554047	
2	-241.7147899470	1402.535	-241.9305783917	22882.112	-241.9420820658	31626.661
3	-241.7150567791	266.832	-241.9321116772	1533.285	-241.9450824114	3000.346
4	-241.7151476805	90.901	-241.9324624924	350.815	-241.9456759472	593.536
5	-241.7151869539	39.273	-241.9325898086	127.316	-241.9458761422	200.195
6	-241.7152065365	19.583	-241.9326473919	57.583	-241.9459630522	86.910
7	-241.7152173957	10.859	-241.9326773309	29.939	-241.9460070367	43.984
8	-241.7152238555	6.460	-241.9326944340	17.103	-241.9460317353	24.699
9	-241.7152278625	4.007	-241.9327048108	10.377	-241.9460465298	14.794
10	-241.7152304160	2.553	-241.9327115109	6.700	-241.9460559750	9.445
11	-241.7152321731	1.757	-241.9327159622	4.451	-241.9460622170	6.242
12	-241.7152333427	1.170	-241.9327190445	3.082	-241.9460664110	4.194
13	-241.7152341862	0.843	-241.9327212187	2.174	-241.9460693805	2.969
14	-241.7152347502	0.564	-241.9327227744	1.556	-241.9460715388	2.158
15	-241.7152351748	0.425	-241.9327239259	1.151	-241.9460731010	1.562
16	-241.7152354393	0.264	-241.9327247497	0.824	-241.9460742689	1.168
17	-241.7152356399	0.201	241.9327253752	0.625	-241.9460751123	0.843
18	-241.7152357976	0.158	-241.9327258109	0.436	-241.9460757466	0.634
19	-241.7152358748	0.077	-241.9327261529	0.342	-241.9460761959	0.449
20	-241.7152359358	0.061	-241.9327263655	0.213	-241.9460765519	0.356

The composition of the optimized orbital basis set at CISD valence correlation calculation are listed in Table II. The total energies of CISD calculated at valence correlation stage was extrapolated as a function of angular momentum up to $l = 500$, using the Schwartz patterns [20] $a(l + 1/2)^{-4}$ leading to deduce the basis set incompleteness error ΔE_μ^{OBI} as shown in Table II.

Composition of orbital basis sets for $Al^+\ {}^1S$, Al^2P^o and $Al^-\ {}^3P$ states and corresponding basis set incompleteness error ΔE^{OBI} (in Ha) for CISD valence calculations.

Species	Basis set	No. of STOs	ΔE^{OBI}
$Al^+\ {}^1S$	13s14p11d8f8g8h7i7k 7l6m5n5o4q4r3t3u2v 2w2x1y1z	121	$-0.00012(1)$
$Al\ {}^2P^o$	15s16p15d13f12g11h9 i9k9l7m7n7o6q6r5t5u 4v4w3x3y2z	168	$-0.000009(1)$
$Al^-\ {}^3P$	16s17p15d15f14g12h 11i11k10l9m9n8o6q6r 6t5u5v4w4x3y3z	186	$-0.000020(1)$

The optimized STOs basis set at SD approximation are used to carry out the corresponding valence correlation FCI calculations, where CISDT for $^2P^o$ state and CISDTQ for ^3P state. The sizes of valence FCI space, the model CI space MCI, and the selected CI space SCI for $^2P^o$ and ^3P states for different excitations are presented in Table III. The details for $Al^{+1}S$ state is not appear in Table III because its FCI calculation is restricted to CISD valence calculation. The estimation of valence FCI truncation energy errors which are based on the Brown formula and modified Brown formula do not exceed $-0.003\ \mu$Ha for Al ^3P state and approximately zero truncation energy error for Al ^2P. The error due to CI by part ΔE^{OBI} are estimated according to sensitivity analysis [18], which lead to $\Delta E_{CIBP} \ll 1\ \mu$Ha.

The CI size of the full CI space FCI, the model space MCI and the selected space SCI, for Al $^2P^o$ and Al$^-$ ^3P states for CI valence calculations.

Species	Excitation	FCI-size	MCI-size	SCI-size
Al ^2P	3	822318	218751	214105
Al ^3P	3	6084171	1351413	287277
	4	676787701	122116782	1339814

The relativistic correction contribution to both IP and EA have been estimated by carried out calculations at relativistic Hartree–Fock level [21] on the related atomic lowest levels ^1S, $^2P_{1/2}$ and $^3P_0$ belonging to ^1S, ^2P and ^3P states respectively. Our result for relativistic contribution to electron affinity is little bit below de Oliveira et al. [7] result, the reason for this difference is due to that in de Oliveira relativistic calculation just including the spin–orbit, Darwin and mass-velocity terms.

Composition of orbital basis sets for $Al^+\ {}^1S$, Al^2P^o and $Al^-\ {}^3P$ states for core-valence and core-core (CVCC) correlation calculations.

Species	Basis set	No. of STOs
$Al^+\ {}^1S$	16s16p16d15f14g14h12i12k10 l8m8n6o6q5r4t4u3v2w2x1y1z	175
Al^2P^o	16s18p16d16f14g14h13i12k10 l8m8n6o5q5r4t4u3v2w2x1y1z	178
$Al^-\ {}^3P$	16s18p16d16f15g14h12i12k10 l9m7n7o5q5r4t4u3v2w2x1y1z	179

The developed STOs for the CVCC correlation component calculations are reported explicitly in Table IV. These basis set are used to calculate the corresponding contribution component of both IP and EA. It is important to mention that the convergence of the CVCC correlation effect as a function of basis set optimization are much slower than that for the valence correlation contribution.

Numerical results of total energies contributions on different levels, HF and CISD and FCI for valence calculations component and the contribution of CVCC component and relativistic correction component and there corresponding contribution to the ionization potential are summarized in Table V. The FCI valence contribution recovers 1.15% of the final value of the predicted IP, while the CVCC correlation reduce the predicted value of IP by 0.044%. The smallest contribution comes from the relativistic effect where gives 0.011%. Our predicted value of IP is exact to two decimal point with respect to experiment.

Similarly, in Table VI, we summarized different energies contributions and the corresponding contributions to electron affinity. The FCI valence contribution recovers 21.6% of the final value of the predicted EA which exceeds the corresponding contribution in IP. The CVCC correlation reduces the predicted value of EA by 3.4% which is also exceeding the corresponding value in IP. In EA calculation the relativistic effect reduces the predicted value of EA by 2.12%, while the later effect increases the predicted value of IP by 0.01%. Our CVCC contribution to EA is -15 meV which is below the corresponding de Oliveira et al. result of -16.17 meV, this attributed to the reason, that in our calculation, both core–valence and core–core correlations are taken together into consideration, while de Oliveira et al. calculations are restricted to the effect of inner shell correlation which was determined as the difference between valence only and all electron CCSD(T) (coupled cluster with all single and double excitations and triple excitations) calculations using the Martin–Taylor family of core-correlation basis sets [7].

As seen from Tables V and VI, it is clear that CVCC component is of negative sign (reduces the ionization potential and electron affinity). Also, it should be noted that the effect of inclusion of CVCC correlation on

both ionization potential and electron affinity are crucial to converge with the last measured EA value by Scheer et al. [8] and the experimental value of ionization potential [22]. However, the CVCC can be positive or negative. Finally, we compare our result with some previous results of theoretical ionization potential and electron affinity calculations as shown in Table VII.

TABLE V

Total energies (in Ha) on different levels of valence calculation, core-valence and core-core (CVCC) and relativistic effect (rel) for $Al^{+\ 1}S$ and Al^2P^o and corresponding ionization potential IP (in meV).

Reference	E ($Al^{+\ 1}S$)	E (Al^2P^o)	IP	IP (exp.)
HF	−241.6746681285	−241.8767049219	5497.703	5985.768c
CISD	−241.7152359492	−241.9327264044	5918.219	
FCI	−241.7152359492	−241.9352770580	5987.626	
FCI+ΔE^{OBI}	−241.715249(1)	−241.935286(1)	5987.51(2)	
a CVCC	−0.405184154	−0.405095171	−2.421	
b rel.	−0.454517980	−0.454542816	0.675	
predicted IP			5985.76(2)	

a, b — The corresponding energies can be calculated by adding the respective HF energy; c — [22].

TABLE VI

Total energies E (in Ha) on different levels of valence calculations, core-valence and core-core (CVCC) and relativistic effect (rel) for $Al^{-\ 2}P^o$ and $Al^{-\ 3}P$ and corresponding electron affinity EA (in meV).

Reference	E ($Al^{+\ 1}S$)	E (Al^2P^o)	IP	IP (exp.)
HF	-241.8767049219	-241.8782311393	41.530	432.83(5)
SD	-241.9327264044	-241.9460765701	363.276	
FCI	-241.9352770580	-241.9520605599	456.702	
FCI+ΔE^{OBI}	-241.935286(1)	-241.952080(1)	456.98(2)	
a CVCC	-0.405095171	-0.404543789	-15.00	
b rel.	-0.454542816	-0.454205563	9.177	
predicted EA			432.81(2)	

a, b — The corresponding energies can be calculated by adding the respective HF energy.

6. Conclusion

We have investigated different contributions to the ionization potential and electron affinity (valence correlation, valence–core and core–core correlation and relativistic effect) of the ground state of aluminum in the frame work of CI. Our calculation includes development of the Slater type orbitals basis set suitable for core–core and core–valence correlation calculations. Our work presents the best result up to date for the ground state of ionization potential and electron affinity of aluminum where FCI truncation energy errors for valence calculation do not exceed −0.003 μHa for Al ^3P state and approximately zero truncation energy error for Al ^2P.

Acknowledgments

TABLE VII

A comparison of previous theoretical and present results of ionization potential IP and electron affinity EA. IP and EA in (meV).

Ref.	Method	IP	EA
Arnau et al. [1]	CI-SP		450
Woon and Dunning [4]	MRSD-CI		437
Eliav et al. [5]	RCC	5991	427
Wijesundera [6]	MCDF		433
de Oliveira et al. [7]	CCSD(T)		432.77
present work	CI-SDT(Q)		432.811
present work	CI-SD(T)	5985.764	

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