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RELATIVISTIC MR-MP ENERGY LEVELS FOR L-SHELL IONS OF SILICON

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Abstract

Level energies are reported for Si V, Si VI, Si VII, Si VIII, Si IX, Si X, Si XI and Si XII. The energies have been calculated with the relativistic Multi-Reference Møller-Plesset Perturbation Theory method and include valence and K-vacancy states with n /up to $5f$. The accuracy of the calculated level energies is established by comparison with the recommended data listed in the National Institute of Standards and Technology (NIST) on-line database. The average deviation of valence level energies ranges from 0.20 eV in Si V to 0.04 eV in Si XII. For K-vacancy states, the available values recommended in the NIST database are limited to Si XII and Si XIII. The average energy deviation is below 0.3 eV for K-vacancy states. The extensive and accurate dataset presented here greatly augments the amount of available reference level energies. We expect our data to ease the line identification of L-shell ions of Si in celestial sources and laboratory generated plasmas, and to serve as energy references in the absence of more accurate laboratory measurements.

Keywords

atomic data; line: identification

1. INTRODUCTION

Spectral lines of L-shell ions of silicon have been observed in many astrophysical objects (see Raassen et al. (2002); Hell et al. (2016) and references in there). The analysis of these spectral lines allows a determination of, among other things, the ionization states, the abundance of elements, the electron temperature, and the density of the astrophysical objects. For instance, K-shell spectral lines of L-shell Si ions have been used to establish the nature of stellar wind in the case of high-mass X-ray binaries (Watanabe et al. 2006; Miškovičová et al. 2016). While the lines of H-like ions are well established, there have been questions on the identification of lines from lower charge states. More importantly, the energy of a given transition must be known very accurately, otherwise it provides only a poor constraint on the flow velocities informed from astrophysical observations, as

illustrated in the case of the K-shell emission or absorption lines of L-shell ions of oxygen (Schmidt et al. 2004; Gu et al. 2005). Generally, the analysis of K-shell spectra demands accurate atomic data such as level energies, wavelengths, radiative rates, Auger rates, and electron impact excitation collision strengths. Many of these atomic parameters have been measured in the laboratory for L-shell Si ions (see Faenov et al. (1994); Kramida & Träbert (1995); Vilkas et al. (2005); Hell et al. (2016) and references in there). Multiple systematic (Behar & Netzer 2002; Gu 2005; Liang et al. 2007; Palmeri et al. 2008; Karim 2011; Wang et al. 2011; Hell et al. 2016) and targeted (Orloski & Trigueiros 2001; Wei et al. 2010; Tayal 2012; Sossah & Tayal 2015; Wei et al. 2014) calculations have complemented the measurements. Atomic data has also been provided by calculations of the isoelectronic sequence of various L-shell ions (Safronova & Shlyaptseva 1996; Jönsson et al. 2011; Rynkunb et al. 2012; Jönsson et al. 2013, 2014; Rynkunb et al. 2014; Nazé et al. 2014; Wang et al. 2014, 2015, 2017).

Most of these calculations focused on valence level energies, and only a limited number of them deals with K-vacancy level energies (Safronova & Shlyaptseva 1996; Behar & Netzer 2002; Palmeri et al. 2008; Wei et al. 2010; Karim 2011; Wang et al. 2011; Wei et al. 2014; Hell et al. 2016). Moreover, valence level energies have been studied to a high level of accuracy with large-scale Relativistic Configuration Interaction (RCI) (Jönsson et al. 2011; Rynkunb et al. 2012; Jönsson et al. 2013, 2014; Rynkunb et al. 2014; Nazé et al. 2014) and combining RCI with Many-Body Perturbation Theory approaches (Vilkas et al. 2005; Wang et al. 2014, 2015). On the other hand, K-vacancy level energies in L-shell Si ions have been studied with small-size semi-relativistic CI (Palmeri et al. 2008) and RCI (Wei et al. 2010, 2014; Wang et al. 2011; Hell et al. 2016) calculations. A result of such disparity in calculations is that the uncertainty in most calculated valence level energies is lower than 0.15 eV, while for K-vacancy levels it is well over 1 eV. Such a large uncertainty constraints the identification of X-ray lines coming from K-vacancy levels of Si ions and their use in velocity determinations via Doppler-Shift measurements.

In this work, we present an accurate and extensive dataset for valence as well as K-vacancy level energies of L-shell ions of Si. The level energies were calculated with the relativistic Multi-Reference Møller-Plesset Perturbation Theory (MR-MP) method (Vilkas et al. 1999; Vilkas & Ishikawa 2005). The MR-MP method has been shown to yield highly accurate valence level energies (Vilkas et al. 2005) and core-excited level energies (Beiersdorfer et al. 2013; Díaz et al. 2013; Beiersdorfer et al. 2017). The work is organized as follows. In Sec. 2, the computational methods are briefly described. The results are shown and discussed in Sec. 3, where our level energies are compared with experimental and previous theoretical values for valence states and K-vacancy states. We conclude in Sec. 4 with a summary.

2. COMPUTATIONAL METHODS

The MR-MP method (Vilkas et al. 1999; Vilkas & Ishikawa 2005) consists of three stages. Initially, a state-averaged Multi-Configuration Dirac-Fock Calculation (MCDF) is performed for the ground and low-lying excited states of the ions to obtain a single set of core and valence spinors in the V^N potential. The single set of spinors was obtained by averaging the

energies of even- and odd-parity states arising from the nonrelativistic configurations $1s^22(s,p)^q$ and $1s^22(s,p)^{q-1}nl$ where $1 \leq q \leq 8$ and $(n \leq 5$ and $l \leq 3)$.

In the second stage, the set of spinors is employed to perform Multi-Reference Configuration Interaction (MR-CI) calculations. For MR-CI, we included all relativistic configurations arising from the following nonrelativistic configurations: $1s^22(s,p)^q$, $1s^22(s,p)^{q-1}nl$, $1s^12(s,p)^{q+1}$, $1s^12(s,p)^qnl$, $2(s,p)^{q+2}$ and $2(s,p)^{q+1}nl$. The levels arising from these configurations can be classified as valence, single K-vacancy, and double K-vacancy levels. After the MR-CI, the CI wavefunction is used as the based for state-specific MR-MP second order perturbation theory calculations. All electrons have been included in the MR-MP calculations to accurately account for relativity and electron correlation effects. Radiative corrections, or the lowest-order quantum electrodynamical (QED) effects, were estimated evaluating (Indelicato et al. 1987) the electron self-energy and vacuum polarization for each state.

In the relativistic MR-MP method, the large and small radial components of the bound Dirac spinors are expanded in sets of even-tempered Gaussian-type functions (Ishikawa et al. 1991). For all systems, we used basis sets of $34s32p30d28f$ Gaussian (G) spinors for angular momentum values up to $L = 3$, 26 G spinors for $L = 4-5$, and 15 G spinors for $L = 6-11$. The parameters α , which define the basis exponents, $\{\zeta_i = \alpha\beta^{i-1}; i = 1, 2, \dots, N_\kappa\}$, is set to $\alpha = 0.000450$ and $\beta = 2.1$.

3. RESULTS AND DISCUSSION

The calculated level energies are given in Table 1. The accuracy of the calculated energies was assessed by comparing our results with the recommended values listed in the NIST on-line database (Kramida et al. 2015). The NIST database lists valence level energies for all L-shell ions of Si. For single K-vacancy level energies, the NIST database only lists entries for Si XII and Si XI. No level energies are listed for double K-vacancy levels. We will first discuss our results for valence levels and afterward the results for single K-vacancy level energies.

3.1. Valence level energies: $1s^22(s,p)^q$ and $1s^22(s,p)^{q-1}nl$

A total of 391 valence level energies were compared with the recommended values available in the NIST database. In an initial analysis, we found that only 13 of these level energies show a deviation above 0.3 eV. We discuss the deviation in these levels later in this section. In Figure 1, we show box-and-whisker plots for the absolute deviation between MR-MP valence level energies and the suggested values listed in the NIST on-line database for L-shell Si ions. In the plot, the lower and upper quartiles are the end of the box, the vertical line inside the box is the median, and the two lines outside the box indicate the highest and lowest absolute deviation. Note that the results in Figure 1 do not include the 13 valence level energies with deviations higher than 0.3 eV. Excluding the 13 levels, the median of the absolute deviation is below 0.25 eV for all ions. In general, the median increases with the number of electrons, going from 0.02 eV in Si XII to 0.21 eV in Si V. The increasing deviation mirrors the higher complexity in the less ionized ions.

We now turn to discuss the 13 levels with a deviation above 0.3 eV. A close inspection of the 13 levels revealed that the source of the deviation of 6 of these levels is easily identified. For Si XI, there are three levels with a significant deviation, the $2s3p^3P_{0,2}^o$ and $2p3s^1P_1^o$ levels (Table 2). The recommended energy value listed in the NIST database of 283.33 eV for the levels $2s3p^3P_{0,1,2}^o$ agrees well only with the MR-MP value for the level $2s3p^3P_1^o$. The $2s3p^1P_{0,1,2}^o$ levels were recently studied base on combined CI and Many-Body Perturbation Theory (MBPT) calculations by Wang et al. (2015). The CI-MBPT values agreed better with the energies recommended by Kramida & Träbert (1995); 283.68, 283.81, 283.90 eV for the $2s3p^3P_{0,1,2}^o$ levels, respectively. The corresponding CI-MBPT values are 283.75, 283.86 and 284.01 eV (Wang et al. 2015). The MR-MP values for the $2s3p^3P_{0,1,2}^o$ levels are 283.73, 283.35, and 283.99 eV, respectively. For the level $2s3p^3P_1^o$ our MR-MP value deviates by almost 0.5 eV from the CI-MBPT result and the recommended value of Kramida & Träbert (1995). In general, the MR-MP and CI-MBPT methods should yield similar results. This is the case for the $2s3p^3P_{0,2}^o$ levels, where MR-MP agrees well with CI-MBPT and the values recommended by Kramida & Träbert (1995). The source of the discrepancy between MR-MP and CI-MBPT for the level $2s3p^3P_1^o$ could be the size of the CI expansion. For instance, our CI expansion includes core-valence correlations while the CI in Wang et al. (2015) only included valence-valence correlations.

In the case of the level $2p3s^1P_1^o$ in Si XI, the large deviation, 1.5 eV, might come from a large uncertainties in the NIST suggested value. Wang et al. (2015) compared CI-MBPT results with the values recommended in the NIST database for the level $2p3s^1P_1^o$ in Be-like Ne, Na, Mg, Al, Si, P, Mn, Fe and Co. Excluding Ne VII, the CI-MBPT values deviated by over 0.3% of the NIST recommended values, that is a deviation of more than 0.5 eV. In Table 3, we have performed a similar analysis but also including low charged Be-like ions. For C III, N IV and O V, MR-MP reproduces the energies from the NIST database within 0.1 eV. In the case of Be-like Mg, Si, Mn and Fe, MR-MP and CI-MBPT deviate from NIST energies by over 0.8 eV. Note that the MR-MP and CI-MBPT values are similar within 0.05 eV. These results corroborate that the deviation for the level $2p3s^1P_1^o$ in Si XI comes from uncertainties in the NIST recommended value.

Another level with a significant deviation is the $2s2p(^1P^o)3p^2S_{1/2}$ level in B-like Si X. The NIST recommended value for this level is 278.51 eV (Table 2). We note that in the NIST database the spectroscopic notation of this energy level had a question mark attached to it. Si X was previously studied with the MR-MP method (Vilkas et al. 2005), and the $2s2p(^1P^o)3p^2S_{1/2}$ level was revised based on wavelength measurements. The energy for this level from wavelength measurements is 279.35 eV (Dere et al. 1997; Del Zanna et al. 2015), which agrees very well with the present MR-MP result of 279.39 eV and the MR-MP calculations by Vilkas et al. (2005) of 279.42 eV. The small difference between the two MR-MP results likely comes from differences in the basis set and the CI expansion. The present MR-MP calculations were performed with a larger basis set and CI expansion than those performed by Vilkas et al. (2005). It seems clear that the NIST value which differs by about 0.9 eV needs to be revised.

The last two levels with significant deviations are the $2s2p^2(^2P)3d^3F_2$ level in C-like Si IX, and the $2s^22p^2(^3P)4s^2P_{3/2}$ level in N-like Si VIII. The recommended energy value listed in the NIST database of 271.63 eV for the $2s2p^2(^2P)3d^3F_{2,3,4}$ levels agree well with the MR-MP value of 271.50 eV for the $2s2p^2(^2P)3d^3F_4$ level. The large error (1.5 eV) in this case results from the incorrect designation of 271.63 eV also to the $2s2p^2(^2P)3d^3F_2$ level. We note that the NIST entry for the $2s2p^2(^2P)3d^3F_{2,3,4}$ levels indicates that the levels may not be real. In the case of the $2s^22p^2(^3P)4s^2P_{3/2}$ level in Si VIII, the large deviation (3.3 eV) likely comes from an incorrect designation. In the NIST database, two energy values, 239.19 and 246.72 eV, are assigned to the $2s^22p^2(^3P)4s^2P_{3/2}$ level. We note that the NIST entry indicates that this level may not be real. However, MR-MP yields an energy of 239.06 eV for the $2s^2_{1/2}2p^2_{3/2}4s_{1/2}$ ($J = 3/2$) level, relatively close to the first value recommended in the NIST database. The MR-MP results for this level agree well with the previous calculation by Orloski & Trigueiros (2001), where a value of 239.16 eV was reported for the $2s^22p^2(^3P)4s^2P_{3/2}$ level.

Table 4 shows the other 7 level energies with a deviation above 0.3 eV. For these level energies, the source of the deviation may come from both uncertainties in the NIST recommended values and limitations in the MR-MP method. We suggest that the differences are due to the uncertainties in the NIST database values because our MR-MP results are in general within 0.25 eV of the NIST recommended values for most levels. At the same time, we recognize that most levels in Table 4 are from the very complex C-, N- and O-like systems, where electron correlation effects are large. The number of configurations included in our MR-MP calculations might not be enough to fully capture such correlation effects in all states. Previous theoretical results also show significant deviations for the levels in Table 4. In the case of the $2p^4^1S_0$ level in Si IX, previous CI-MBPT (Wang et al. 2014) and FAC (Wei et al. 2014) calculations yielded values of 101.42 and 104.63 eV, respectively, deviating by -0.2 eV and 3 eV from the value suggested in the NIST database. Previous calculations (Orloski & Trigueiros 2001; Bhatia & Landi 2003; Tayal 2012; Nazé et al. 2014; Wang et al. 2017) for the $2s2p^4^2P_{1/2}$ level in Si VIII yielded values that overestimated the NIST recommended values from 0.22 to 4.19 eV.

In the case of the $2p^6^1S_0^o$ level in O-like Si VII, a previous MR-MP value (Vilkas et al. 1999) is 104.75 eV, deviating by -0.52 eV from the suggested value in the NIST database. Values of 105.39 and 105.64 eV were reported by Sossah & Tayal (2015) and Froese Fischer & Tachiev (2004), respectively. As mentioned above, the difference between the two MR-MP results is due to differences in the basis set and the CI expansion. The possible limitations of the present MR-MP calculations to fully treat electron correlation effects can be seen by inspecting the $2p^6^1S_0^o$ level in other O-like ions. We include in Table 5 MR-MP level energies for $2p^6^1S_0^o$ in Ne III, Mg V, Si VII, Ar XI, Mn XVIII, and Fe XIX. The deviation decreases smoothly with increasing atomic number Z . This is the expected behavior because electron correlation effects play a major role in low- Z ions (Vilkas et al. 1999). The deviations seen in Table 4 come in part from an incomplete treatment of electron correlation in our MR-MP calculations. Nevertheless, our MR-MP valence level energies are

highly accurate. We will turn now to a discussion of the MR-MP results for the single K-vacancy level energies.

3.2. K-vacancy level energies: $1s^12(s,p)^{q+1}$ and $1s^12(s,p)^q nl$

As mentioned previously, the NIST database only recommends K-vacancy level energies for Si XII and Si XI. The NIST database lists 16 K-vacancy level energies belonging to the configurations $1s2s^2$, $1s2s2p$ and $1s2p^2$ for Si XII (Table 6), and 13 K-vacancy levels with configurations $1s2s^22p$, $1s2s2p^2$ and $1s2p^3$ for Si XI (Table 7). The suggested values in the NIST database are compared with our MR-MP results in Figure 2. We also included in Figure 2 the deviation between the NIST recommended values and previous HFR (Palmeri et al. 2008), FAC (Hell et al. 2016; Wei et al. 2010) and AUTOSTRUCTURE (Del Zanna et al. 2015) calculations. For Si XII, the MR-MP K-vacancy level energies are within 0.3 eV of the recommended values in the NIST database while the other methods are within 1 eV. In the case of Si XI, the MR-MP results are within 0.6 eV of the NIST recommended values. The other methods deviate by over 1 eV, particularly for the $1s2p^3$ levels, i.e. the last three levels in Table 7. Other previous calculations (data not included here), based on relativistic MCDF (Sang et al. 2016) and Z-expansion theory (Safronova & Shlyaptseva 1996), also show a significant deviation from NIST for the $1s2p^3$ levels. The MR-MP method reproduces the NIST recommended values much better than the previous calculations. A closer look at the comparison of the MR-MP and the NIST recommended values for Si XI reveals that only 4 K-vacancy level energies deviate by more than 0.3 eV, the energies of the other 9 levels are within 0.2 eV; see Table 7.

4. SUMMARY

In summary, we have calculated valence and K-vacancy level energies of L-shell ions (Li - Ne) of Si. In general, the absolute deviation from available measurements is below 0.3 eV for both valence and K-vacancy level energies. In a small number of cases, the level energies can have a deviation in the range of 0.3 – 0.6 eV. We hope more measurements become available in near future, particularly for K-vacancy level energies, so that computational methods to study high excited states can be further improved. Nevertheless, the present dataset is highly accurate, and our energy values may serve as reference values for Doppler-Shift measurements. Moreover, the present dataset will be of great help in line identification and for confirming level designations.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

Box-and-whisker plots for the absolute deviation between MR-MP valence level energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for L-shell ions of Si. The number of level energies that were included in the statistical analysis is given above each box.

Figure 2.

Deviation between MR-MP energies and the recommended values in the NIST on-line database (Kramida et al. 2015) for K-vacancy states in (a) Si XII and (b) Si XI. The level index in the x -axis corresponds to levels in Tables 6 and 7. Previous calculations with various codes are also included for comparison: HFR (Palmeri et al. 2008), FAC1 (Wei et al. 2010), FAC2 (Hell et al. 2016), and AUTOSTRUCTURE (as included in the CHIANTI v8 data base (Dere et al. 1997; Del Zanna et al. 2015)).

Table 1

Valence level energies in L-shell ions of Si evaluated with the MR-MP method.

<i>N</i>	Index	Configuration ^{a,b}	<i>J</i>	Parity	Energy (eV)
3	1	1s22s	1/2	even	0.00
3	2	1s22p−	1/2	odd	23.82
3	3	1s22p+	3/2	odd	24.83
3	4	1s23s	1/2	even	296.23
3	5	1s23p−	1/2	odd	302.78
3	6	1s23p+	3/2	odd	303.08
3	7	1s23d−	3/2	even	305.48
3	8	1s23d+	5/2	even	305.58
3	9	1s24s	1/2	even	397.03
3	10	1s24p−	1/2	odd	399.73
3	11	1s24p+	3/2	odd	399.86
3	12	1s24d−	3/2	even	400.85
3	13	1s24d+	5/2	even	400.89
3	14	1s24f−	5/2	odd	400.94
3	15	1s24f+	7/2	odd	400.96
3	16	1s25s	1/2	even	443.07
3	17	1s25p−	1/2	odd	444.49
3	18	1s25p+	3/2	odd	444.55
3	19	1s25d−	3/2	even	445.03
3	20	1s25f−	5/2	odd	445.04
3	21	1s25f+	7/2	odd	445.05
3	22	1s25d+	5/2	even	445.05

Note—Note that only 22 levels arising from the $1s^2nl(n-5 \text{ and } l-3)$ configurations in Si XII ($N=3$) are shown here.

^a $s = s1/2$, $p = p1/2$, $p+ = p3/2$, $d = d3/2$, $d+ = d5/2$, $f = f5/2$ and $f+ = f7/2$.

^b The number after the $-/+$ symbols is the power of the corresponding configuration. For example, the jj configuration of level 15 is $1s^2_{1/2}4f_{7/2}$ (Table 1 is published in its entirety in the machine-readable format. A portion is shown here for guidance regarding its form and content.)

Table 2

Valence level energies (eV) of L-shell ions of Si with a significant deviation between the NIST recommended values and our MR-MP results.

Ion	Level	NIST	MR-MP	Deviation
Si XI	$2s3p\ ^3P_0^o$	283.33	283.73	0.40
	$2s3p\ ^3P_2^o$	283.33	283.99	0.66
	$2p3s\ ^1P_1^o$	306.34	304.84	-1.50
Si X	$2s2p(^1P^o)3p\ ^2S_{1/2}$	278.51	279.39	0.88
Si IX	$2s2p^2(^2P)3d\ ^3F_4$	271.63	270.09	-1.54
Si VIII	$2s^22p^2(^3P)4s\ ^2P_{3/2}$	246.72	243.47	-3.25

Table 3

Energy (eV) of the $2p3s^1P_1^o$ level in various Be-like ions. CI-MBPT results from Wang et al. (2015) are included for comparison.

Ion	NIST	MR-MP	CI-MBPT
C III	38.44	38.45	–
N IV	58.65	58.55	–
O V	82.39	82.29	–
Ne VII	141.20	141.13	–
Mg IX	216.11	215.25	215.24
Si XI	306.34	304.85	304.84
Mn XXII	1078.91	1084.08	1084.13
Fe XXIII	1174.1	1180.03	1180.08

Table 4

Valence level energies (eV) of L-shell ions of Si with a deviation between the NIST recommended values and the MR-MP results of 0.3 – 0.5 eV.

Ion	Level	NIST	MR-MP	Deviation
Si IX	$2p^4\ ^1S_0$	101.63	102.02	0.39
Si VIII	$2s2p^4\ ^2P_{1/2}$	66.06	66.48	0.42
Si VII	$2p^6\ ^1S_0^o$	105.27	105.64	0.37
	$2s^22p^3(^2P^o)4s\ ^3P_2^o$	207.04	206.58	−0.46
	$2s^22p^3(^2P^o)5s\ ^1P_1^o$	227.86	227.38	−0.48
	$2s2p^4(^4P)4s\ ^3P_2$	234.04	233.68	−0.36
Si V	$2s^22p^5(^2[P]_{1/2}^o)4p\ _{2[1/2]_0}$	141.96	141.61	−0.35

Table 5

Energy (eV) of the $2p^6\ ^1S_0^o$ level in various O-like ions.

Column	NIST	MR-MP	Deviation (eV)
Ne III	59.37	60.61	1.24
Mg V	82.20	82.72	0.52
Si VII	105.27	105.64	0.37
S IX	128.85	129.12	0.27
Ar XI	153.19	153.41	0.21
Mn XVIII	248.90	249.06	0.16
Fe XIX	264.60	264.70	0.10

K-vacancy level energies (eV) of Si XII recommended in the NIST database. Our MR-MP results and previous calculations are included for comparison: FAC2 (Hell et al. 2016), HFR (Palmeri et al. 2008), and AUTOSTRUCTURE (AS) (as included in the CHIANTI v8 data base (Dere et al. 1997; Del Zanna et al. 2015)).

Table 6

Index	Configuration	NIST	MR-MP	FAC2	HFR	AS
1	$1s2s^2S_{1/2}$	1820.44	1820.39	1819.37	1819.76	1819.98
2	$1s2s^2P^o_{1/2}$	1826.57	1826.28	1825.60	1825.64	1824.60
3	$1s2s^2P^o_{3/2}$	1826.83	1826.55	1825.87	1826.05	1825.00
4	$1s2s^2P^o_{5/2}$	1827.52	1827.23	1826.55	1826.78	1825.69
5	$1s2s^2P^o_{1/2}$	1844.99	1844.80	1844.29	1844.79	1844.37
6	$1s2s^2P^o_{3/2}$	1845.54	1845.36	1844.86	1845.33	1844.90
7	$1s2p^4P_{1/2}$	1851.93	1851.65	1851.48	1851.17	1851.43
8	$1s2p^4P_{3/2}$	1852.37	1852.11	1851.88	1851.61	1851.85
9	$1s2p^4P_{5/2}$	1852.88	1852.62	1852.41	1852.29	1852.51
10	$1s2p^4P^o_{1/2}$	1853.57	1853.37	1853.91	1853.90	1852.44
11	$1s2p^4P^o_{3/2}$	1853.83	1853.56	1854.09	1854.22	1852.72
12	$1s2p^2D_{3/2}$	1863.82	1863.63	1864.35	1863.97	1863.62
13	$1s2p^2D_{5/2}$	1863.96	1863.78	1864.48	1864.08	1863.53
14	$1s2p^2P_{1/2}$	1866.86	1866.82	1867.12	1866.94	1866.98
15	$1s2p^2P_{3/2}$	1867.82	1867.79	1868.08	1867.89	1867.90
16	$1s2p^2S_{1/2}$	1880.54	1880.32	1881.32	1881.21	1880.33

K-vacancy level energies (eV) of Si XI recommended in the NIST database. Our MR-MP results and previous calculations are included for comparison: FAC1 (Wei et al. 2010) and HFR (Palmeri et al. 2008). NIST values with a deviation from MR-MP over 0.3 eV are highlighted in *italic*.

Table 7

Index	Configuration	NIST	MR-MP	FAC1	HFR
1	$1s^2 2p^3 \ ^1P^o_1$	<i>1828.62</i>	1829.21	1827.54	1828.89
2	$1s^2 2p^2 \ ^3D_3$	1844.45	1844.56	1844.19	1845.34
3	$1s^2 2p^2 \ ^3P_0$	1844.82	1844.93	1844.21	1845.12
4	$1s^2 2p^2 \ ^3D_1$	1844.65	1844.94	1844.20	1845.13
5	$1s^2 2p^2 \ ^3P_1$	1845.23	1845.11	1844.71	1845.62
6	$1s^2 2p^2 \ ^3D_2$	<i>1844.56</i>	1845.14	1844.21	1845.19
7	$1s^2 2p^2 \ ^3P_2$	<i>1845.82</i>	1845.43	1845.24	1846.18
8	$1s^2 2p^2 \ ^1D_2$	1858.56	1858.54	1858.63	1859.67
9	$1s^2 2p^2 \ ^3P_2$	1859.67	1859.85	1859.90	1861.22
10	$1s^2 2p^2 \ ^1P_1$	1867.45	1867.66	1867.91	1869.04
11	$1s^2 p^3 \ ^1D^o_2$	<i>1881.62</i>	1881.95	1883.12	1883.18
12	$1s^2 p^3 \ ^3P^o_2$	1883.21	1883.15	1884.45	1884.56
13	$1s^2 p^3 \ ^1P^o_1$	1892.24	1892.47	1894.08	1894.06