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Large-Scale Relativistic Calculations for Atomic Structure and Electron Impact Excitation of Impurity Ions

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Spectroscopic and EIE results

- **Na-like ions of Ar, Kr and Xe**
- **B-like Xe**
- **Ar-like Kr ions**

Extended calculations of Atomic Structure Parameters for Na-like Ar, Kr and Xe Ions using relativistic MCDHF and MBPT Methods

- Highly charged ions of inert gases are of particular interest in plasma research and extreme ultraviolet lithography.
- The spectroscopic data of HCIs of Ar, Kr and Xe are essential to interpret the spectra correctly and to model the conditions in plasmas containing these species.
- There is scarcity of the atomic structures data for higher excited states of Na-like Ar, Kr and Xe ions.
- For Ar^{7+}, fine structure energies and radiative parameters of a few higher levels, viz., $7f$, $7g$, $7i$, $8p$, $8f$, $8g$, $8i$ are absent in the literature.
- For Kr^{25+}, these parameters are available for $n = 3-6$, $l = s, p, d, f$ levels only.
- For Xe^{43+} although its level energies are available up to $n = 3-6$, $l = s, p, d, f$, transition probabilities have been reported for only a few transitions among the low lying states.

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Atomic Structure Parameters for Na-like Ar, Kr and Xe Ions using relativistic MCDHF and MBPT Methods

- Extensive calculations of energies and lifetime of lowest 71 states of Na-like Ar^{7+}, Kr^{25+} and Xe^{43+} ions.
- Radiative parameters viz., wavelengths, line strengths and transition rates among the 71 levels are determined.
- The configurations of interest include: $1s^2 2s^2 2p^6 nl$ for n =3 to 9, l =0 to 6.
- The fully relativistic multiconfiguration Dirac Hartree-Fock (MCDHF) with the Breit and QED (vacuum polarization and self-energy) effects is implemented.
- The effects of the Breit and QED (vacuum polarization and self-energy) corrections on the level energies is analyzed for Xe^{43+}.
- Accuracy of the results are verified by carrying out similar calculations using the many body perturbation theory.

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Multiconfiguration Dirac-Fock (MCDF)

In MCDF, the atomic state is represented by atomic state function (ASF) which is approximated by the linear combination of orthonormal set of configuration state functions (CSFs) having same parity P and angular momentum J

$$\Psi(PJM) = \sum_{i=1}^{n} a_i \, \Phi_i(PJM)$$

$$\sum_{i=1}^{n} a_i^2 = 1$$

$$\Phi_{a(b)}(\mathbf{1}, \mathbf{2}, \mathbf{3}, \ldots, \boldsymbol{n}) = \frac{1}{\sqrt{(n!)}} \begin{Bmatrix} 1s\frac{1}{2}\frac{1}{2} & \ldots n\kappa m \end{Bmatrix}$$

Slater determinant of single electron Dirac-Fock orbitals

Single electron central field Dirac orbitals

$$\phi_{n\kappa m}(\boldsymbol{r}) = \frac{1}{r} \begin{pmatrix} g_\kappa(r)\, \chi_\kappa^m(\hat{\boldsymbol{r}}) \\ i f_\kappa(r)\, \chi_{-\kappa}^m(\hat{\boldsymbol{r}}) \end{pmatrix}$$

Methodology:

MR set: $1s^2 2s^2 2p^6 nl$ for n =3 to 9, l =0 to 6

Odd Set

Even set

Single-double excitation

Core –valence correlation
$1s^2$ is kept inactive

Restricted active space

Active sets:
AS10= 10s, 10p, 10d, 10f, 10g, 10h, 10i
AS11=11s, 11p, 11d, 11f, 11g, 11h, 11i

Number of CSFs

Active set	Even	Odd
AS10	53,352	47,191
AS11	71,820	63,339

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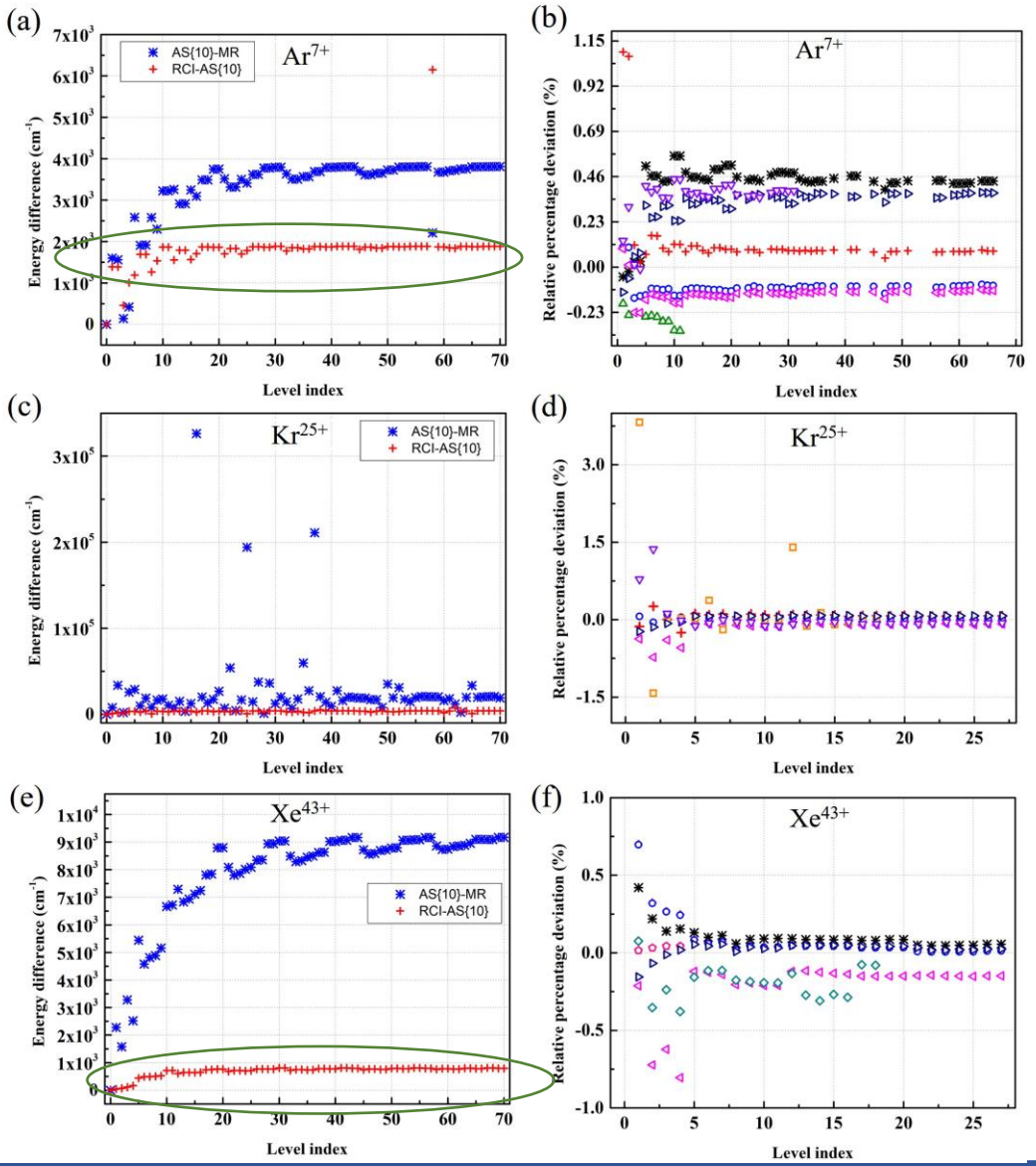
Results



The convergence of present results with increasing active sets for Ar^{7+}, Kr^{25+} and Xe^{43+} , respectively is shown in Figs. (a), (c) and (e).

The comparison of present results with data available from the NIST and other theoretical results is shown in Figs. (b), (d) and (f), respectively..

- The mean relative deviation of the present results with respect to the NIST ASD is 0.15%, 0.032% and 0.08%, respectively for Ar^{7+}, Kr^{25+} and Xe^{43+}.

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The RSCF and RCI energies with contributions from the Breit, self energy (SE), vacuum polarization (VP) and Nuclear corrections for Xe^{43+}

Level	Energies (cm^{-1})						
	RSCF	SE	VP	Nuclear Recoil	Breit	Total	NIST [48]
$3p\ ^2P_{1/2}$	808,702	−19,696	1779	−64	10,643	801,364	806,985
$3p\ ^2P_{3/2}$	1,512,126	−18,236	1855	−63	797	1,496,479	1,501,276
$3d\ ^2D_{3/2}$	2,539,364	−20,144	1857	−86	−4016	2,516,975	2,523,660
$3d\ ^2D_{4/2}$	2,700,953	−19,679	1855	−87	−10,160	2,672,882	2,679,380
$4s\ ^2S_{1/2}$	12,277,698	−16,315	1083	−49	−9534	12,252,883	12,263,000
$4p\ ^2P_{1/2}$	12,611,836	−19,865	1797	−74	−5238	12,588,456	12,596,000
$4p\ ^2P_{3/2}$	12,897,971	−19,591	1829	−74	−9194	12,870,941	12,880,000

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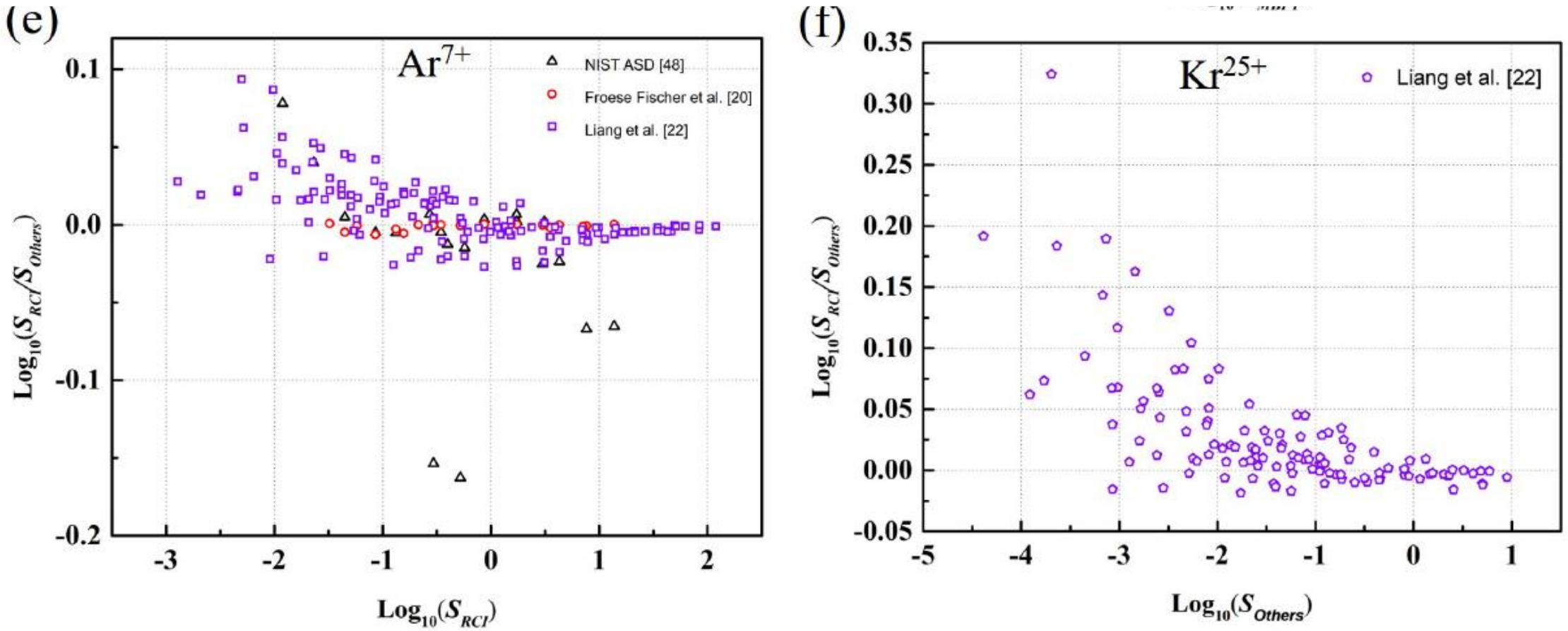
The SE and Breit effects plays a significant role in improving the RSCF energies.

Total represent the sum of all the corrections and the RSCF energies.

Transition parameters

The agreement between the present and others results



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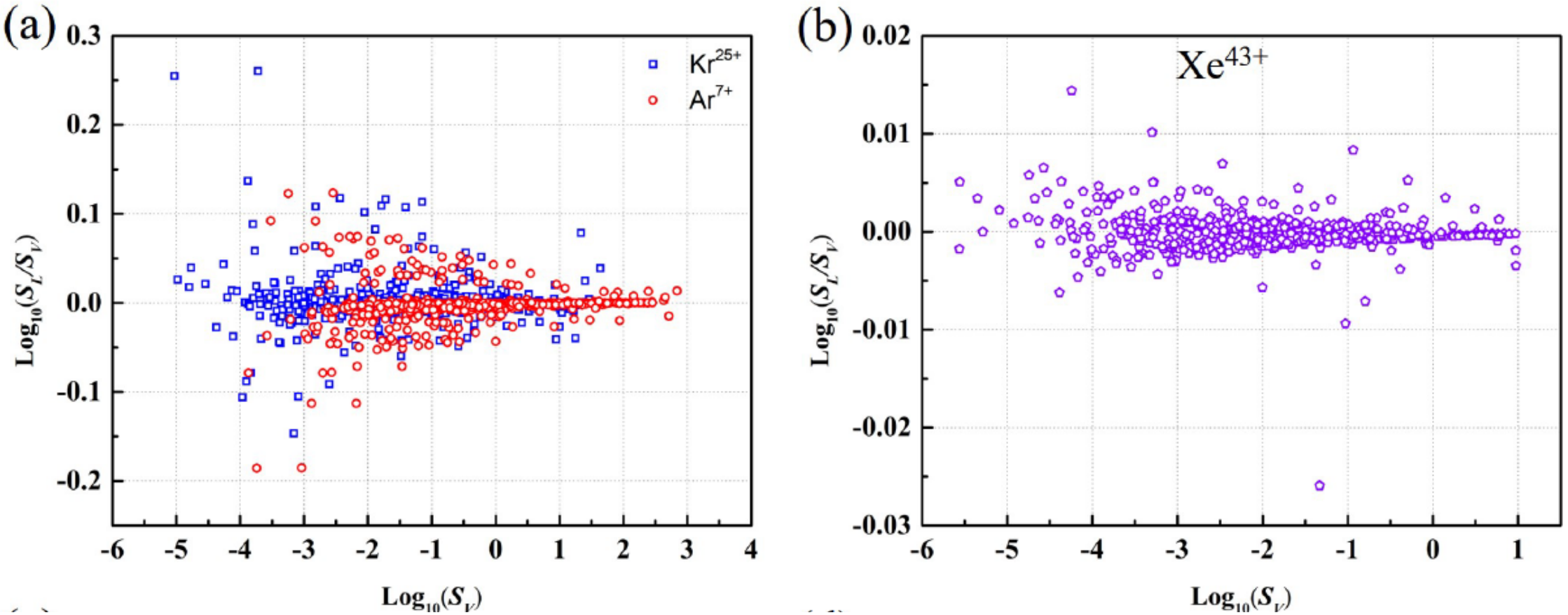
Transition parameters

The agreement between the line strengths (S) calculated in length (S_L) and velocity (S_V) gauges



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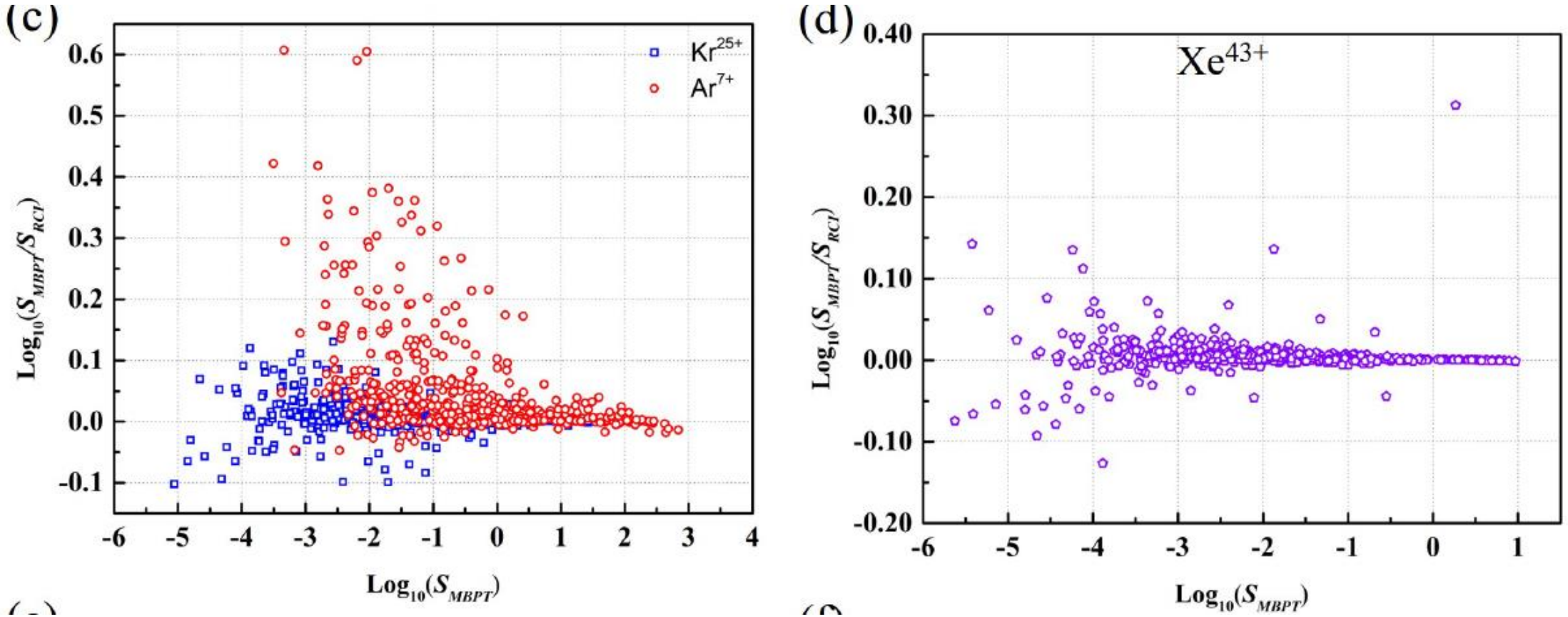
Transition parameters

The relationship between the line strengths from the MCDHF (S_{RCI}) and MBPT (S_{MBPT}) method



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A statistical approach is used to calculate the uncertainty percentage in *S* and transition rates (*A*).

Independent calculations are done for levels with *n* <=7 and *n*>7.

The percentage of transition categorized according to NIST nomenclature

Accuracy	Percentage of E1 transitions					
	$n \leq 7$			$n > 7$		
	Ar^{7+}	Kr^{25+}	Xe^{43+}	Ar^{7+}	Kr^{25+}	Xe^{43+}
A+ ≤ 2%	0	7.48	27.31	0	0	0
A ≤ 3%	0	13.72	4.83	0	0.42	0
B+ ≤ 7%	14.20	15.38	6.93	0	18.30	35.08
B ≤ 10%	12.92	2.70	1.68	2.33	15.59	11.76
C+ ≤ 18%	14.19	2.49	2.10	6.78	14.55	6.09
C ≤ 25%	1.91	0.83	0.42	9.53	4.37	1.47
D+ ≤ 44%	1.91	0.83	0.21	9.32	1.45	1.89
D ≤ 54%	0	0.21	0	5.08	0	0
E > 54%	1.06	0	0	20.76	1.66	0.21

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Electron Impact Excitation

In Relativistic Distorted Wave (RDW) theory, the **Transition matrix** for the electron impact excitation of N-electron atom from initial state $(a) \rightarrow$ final state (b)

$$\boldsymbol{T_{a\rightarrow b}} = \left\langle \Psi_b(\mathbf{1},\mathbf{2},\ldots,\boldsymbol{N}) F_b^{DW-}(\boldsymbol{k_b},\boldsymbol{N}+\mathbf{1}) \middle| V_{in} - U_d(N+1) \middle| \boldsymbol{A}\, \Psi_a(\mathbf{1},\mathbf{2},\ldots,\boldsymbol{N}) F_a^{DW+}(\boldsymbol{k_a},\boldsymbol{N}+\mathbf{1}) \right\rangle$$

- $\Psi_{a(b)}$ Target atom wave function before(after) scattering
- V_{in} Interaction potential
- U_d Distortion potential
- $F_{a(b)}^{DW+(-)}$ Projectile electron distorted wave function

$$V_{in}(r_i, r_j) = V^{Coulomb} + V^{Breit}$$
$$= \sum_{i<j} \left(\frac{1}{r_{ij}} - \alpha_i \cdot \alpha_j \frac{1}{r_{ij}} + \frac{1}{2} (\alpha_i \cdot \nabla_i)(\alpha_j \cdot \nabla_j) r_{ij} \right)$$

Linear Polarization of emitted Photon

Polarization of emitted photons

$$\boldsymbol{P = \frac{3(\sigma_{3/2} - \sigma_{1/2})}{5\sigma_{1/2} + 3\sigma_{3/2}}}$$

$\sigma_{1/2}$ and $\sigma_{3/2}$ represents the excitation to magnetic sub-levels $M_b = 1/2$ and $3/2$ of $(n+1)p_{3/2}$ level from the ground state $ns_{1/2}$, respectively.

Fe^{25+}				
Energy (keV)	**Interaction**	**RDW**	**RCCC [1]**	**Experiment[2]**
30	Coulomb	0.186	0.186	0.071 ± 0.034
30	Coulomb + Breit	0.146	0.145	
120	Coulomb	0.011	0.0095	-0.236 ± 0.109
120	Coulomb + Breit	-0.105	-0.114	

[1] Bostock, Christopher J., Dmitry V. Fursa, and Igor Bray. *Physical Review A* 80.5 (2009): 052708.
[2] Robbins, D. L., et al. *Physical Review A* 74.2 (2006): 022713.

Cross Sections and Rate coefficients

- The scattering amplitude for the transition can be obtained as

$$f(J_b M_b, k_b \mu_b; J_a M_a, k_a \mu_a, \theta) = (2\pi)^2 \sqrt{\frac{k_b}{k_a}} T_{a\to b}(J_b M_b, k_b \mu_b; J_a M_a, k_a \mu_a, \theta)$$

- The Differential Cross Section (DCS) can be calculated from the scattering amplitude as

$$\frac{d\sigma_{a\to b}}{d\Omega} = \frac{1}{2(2J_a+1)} \sum_{\substack{M_a,\,\mu_a \\ M_b,\,\mu_b}} |f(J_b M_b, k_b \mu_b; J_a M_a, k_a \mu_a, \theta)|^2$$

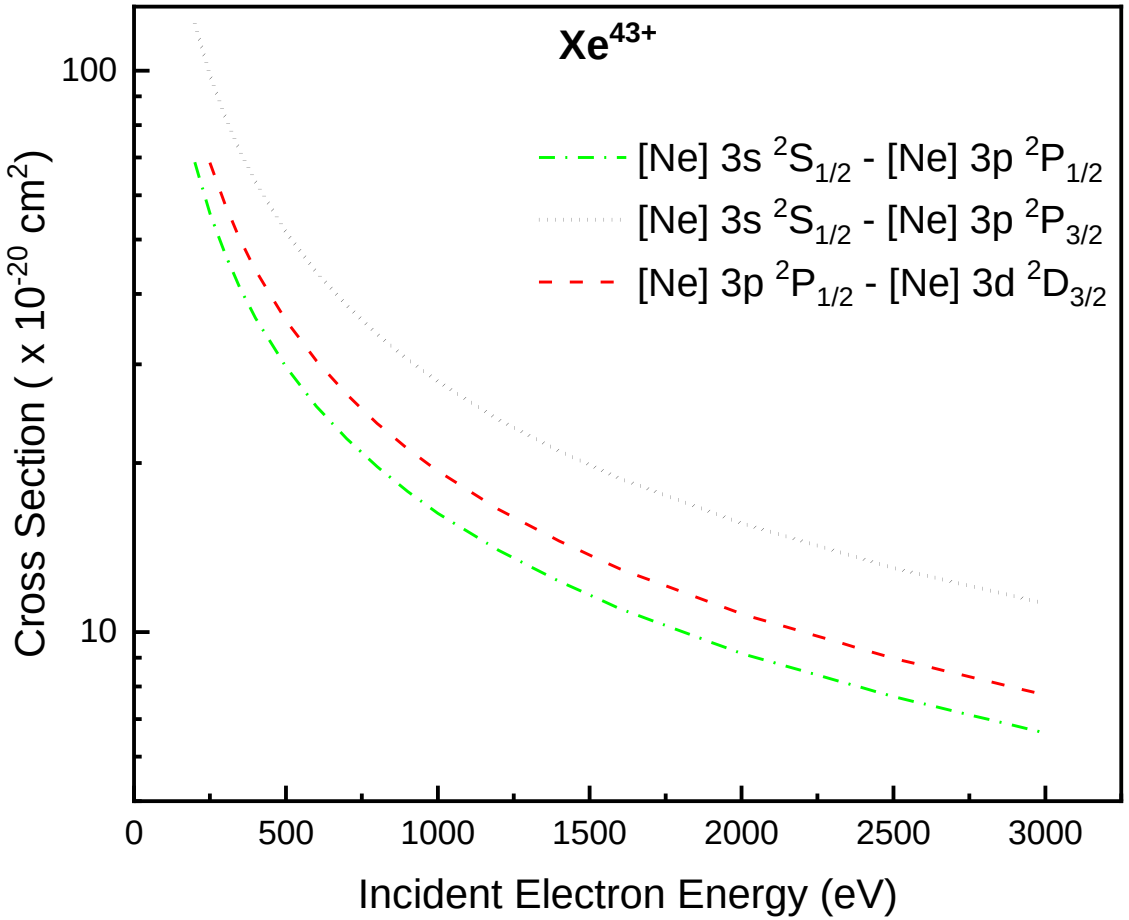
- The Integral Cross Section is calculated by integrating the DCS over all solid angles

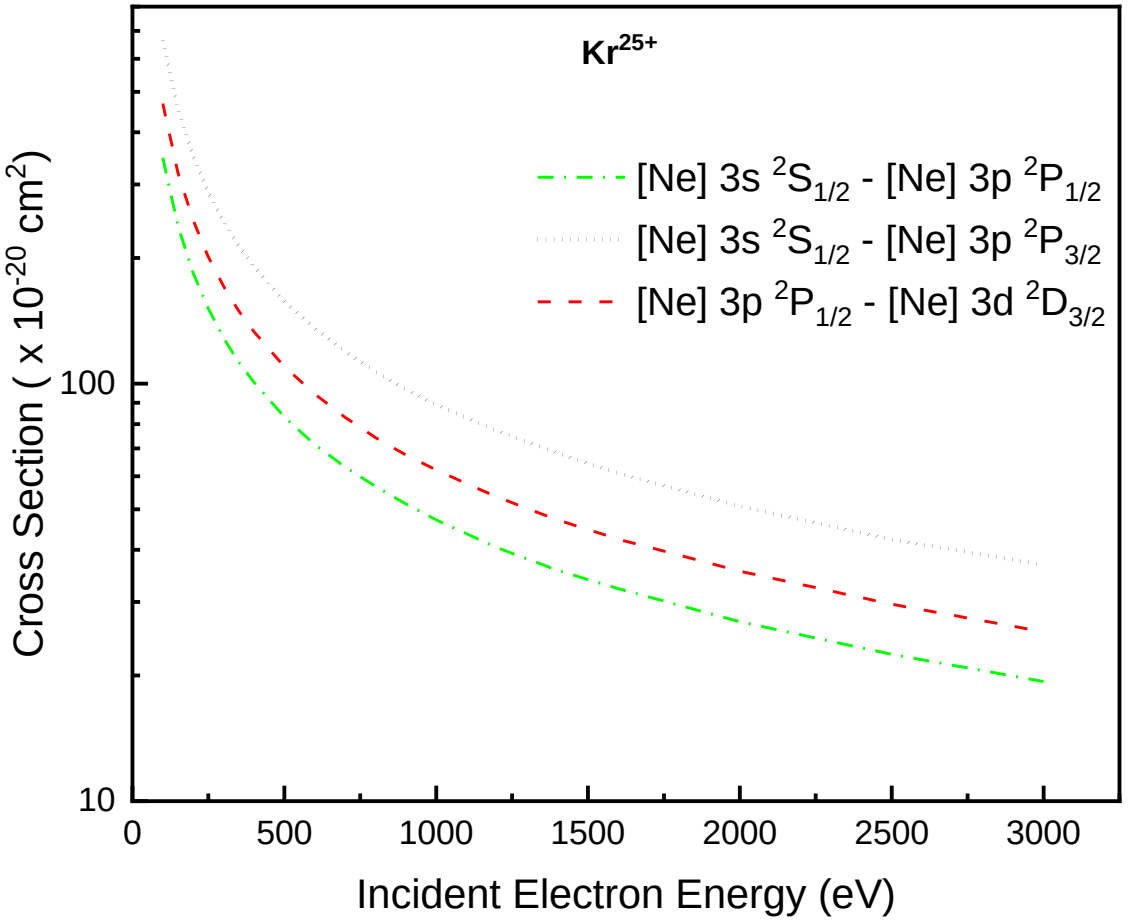
$$\sigma_{a\to b} = \int \frac{d\sigma_{a\to b}}{d\Omega} d\Omega$$

- Rate coefficients $(k_{a\to b})$ at a particular temperature T (considering Maxwellian electron energy distribution function)

$$k_{a\to b} = 2\left(\frac{2}{\pi m_e}\right)^{\frac{1}{2}} (k_B T)^{-\frac{3}{2}} \int_{E_{ab}}^{\infty} E\sigma_{a\to b}(E) exp\left(-\frac{E}{k_B T}\right) dE$$

ICS for Na-like Xe and Kr





Relativistic atomic structure calculations for B-like xenon ions

- Energies and lifetimes of 255 levels of Xe^{49+} are calculated implementing the MCDHF method.
- The electric dipole (E1) and quadrupole (E2), magnetic dipole (M1) and quadrupole (M2) transition parameters among these levels are calculated.
- The configurations under considerations are $1s^2 2s^2 nl$, $1s^2 2p^2 nl$, $1s^2 2s2pnl$ with $n < 5$ and $l = s, p, d, f$.
- Analysis of corrections due to the Breit and QED effects is done for the lowest 15 levels.
- Uncertainties in the lifetimes and line strengths are calculated and transitions are classified according to the NIST accuracy nomenclature.
- Atomic structure parameters for additional 130 levels are reported for the first time.

Methodology

MR set: $1s^2 2s^2 nl$, $1s^2 2p^2 nl$, $1s^2 2s2pnl$ with $n = 2$ *to* 4 and $l = s, p, d, f$.

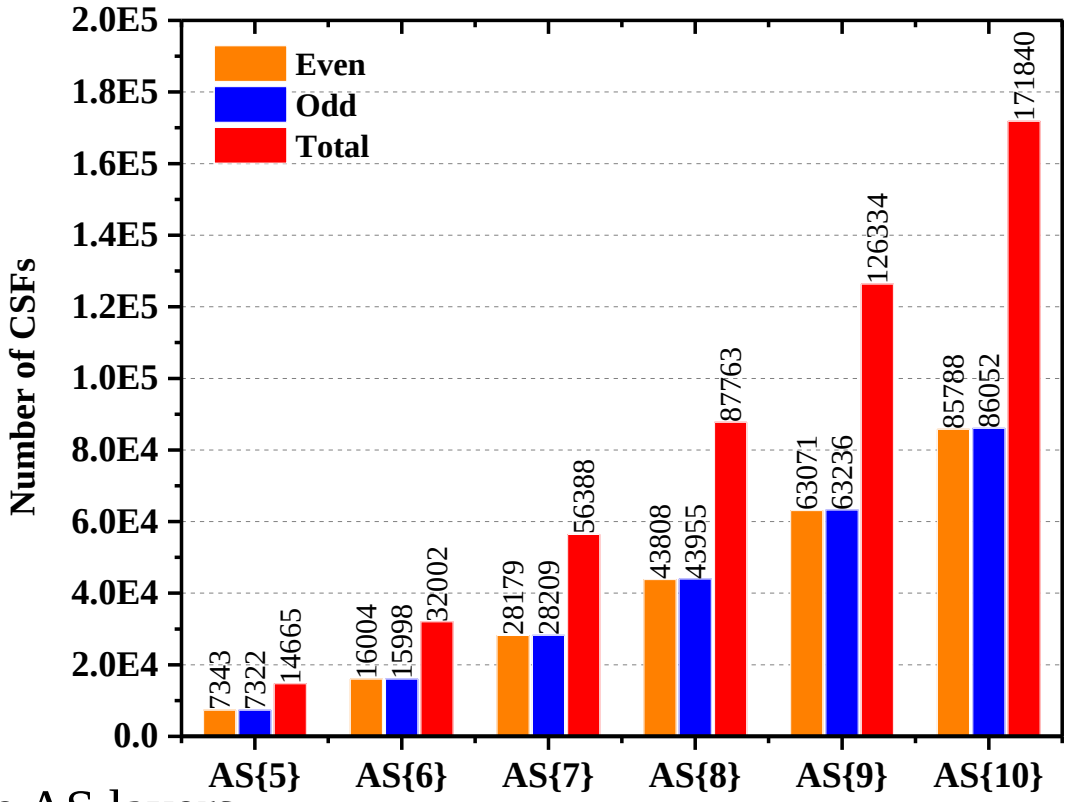
→ 255 levels → Even set 131 levels; Odd set 124 levels

Relativistic self-consistent field (RCSF)

&

Restrictive active space approach:

AS{5} = MR + {5*s*, 5*p*, 5*d*, 5*f*}
AS{6} = AS{5} + {6*s*, 6*p*, 6*d*, 6*f*}
AS{7} = AS{6} + {7*s*, 7*p*, 7*d*, 7*f*}
AS{8} = AS{7} + {8*s*, 8*p*, 8*d*, 8*f*}
AS{9} = AS{8} + {9*s*, 9*p*, 9*d*, 9*f*}
AS{10} = AS{9} + {10*s*, 10*p*, 10*d*, 10*f*}



Correlations: Core-Valence (CV):
Single-Double substitution of electrons from the MR to the AS layers.

1s: Inactive core

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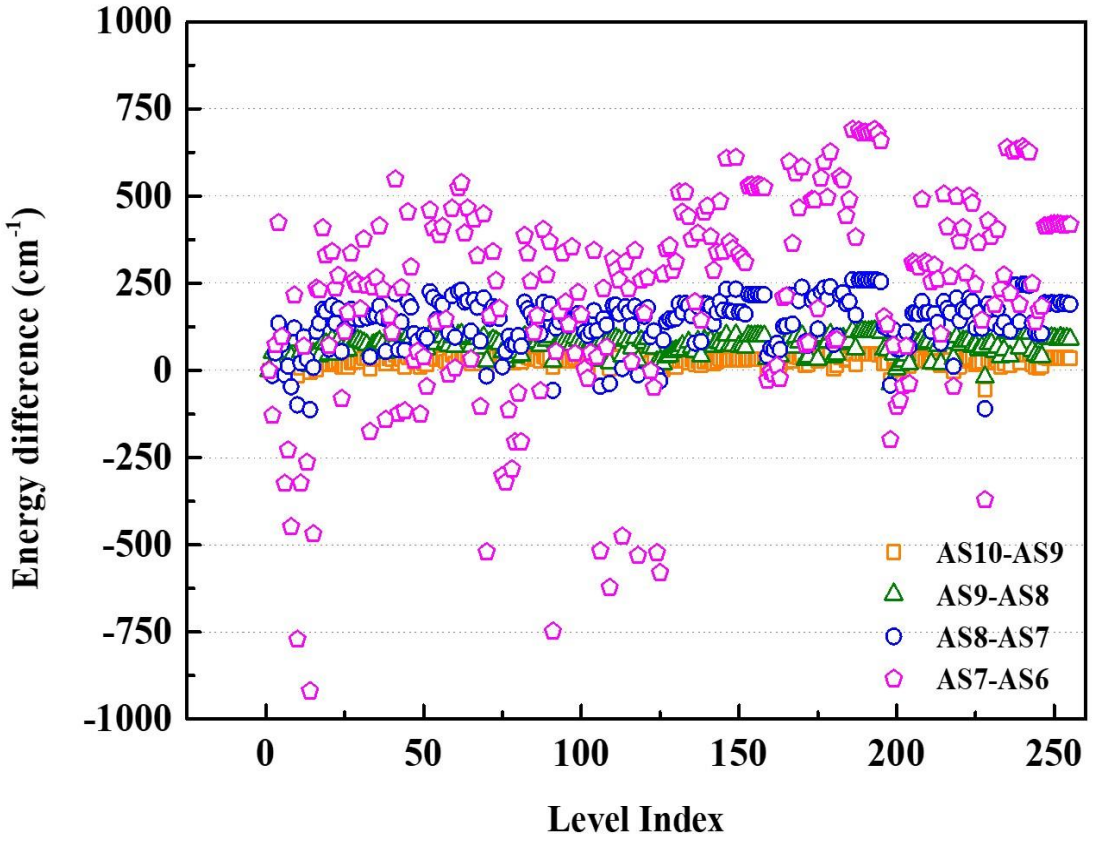
Results

The convergence of present energies with increasing active layers



The present energies (eV) and contribution of Breit and QED corrections

Level	MCDHF	Breit	SE	VP	Total
$2s^2 2p\ ^2P_{1/2}$	0.0	0.0	0.0	0.0	0.0
$2s2p^2\ ^4P_{1/2}$	163.0	6.7	-7.1	0.9	163.5
$2s^2 2p\ ^2P_{3/2}$	363.9	-5.8	0.4	0.1	358.6
$2s2p^2\ ^4P_{3/2}$	477.5	0.8	- 6.5	0.9	472.6
$2s2p^2\ ^2D_{5/2}$	513.1	- 3.1	- 6.5	0.9	504.4
$2s2p^2\ ^2D_{3/2}$	561.5	-1.3	-6.5	0.9	554.6
$2s2p^2\ ^2P_{1/2}$	559.4	1.1	-6.5	0.9	554.9
$2p^3\ ^2D_{3/2}$	735.2	6.1	-13.5	1.8	729.6
$2s2p^2\ ^4P_{5/2}$	861.5	-7.0	-6.0	1.0	849.4
$2s2p^2\ ^2S_{1/2}$	931.4	-3.2	-6.0	1.0	923.2
$2s2p^2\ ^2P_{3/2}$	935.4	-6.0	- 6.0	1.0	924.4
$2p^3\ ^4S_{3/2}$	1067.0	0.7	-13.1	1.9	1056.5
$2p^3\ ^2D_{5/2}$	1090.5	-3.1	-13.1	1.9	1076.1
$2p^3\ ^2P_{1/2}$	1123.7	1.9	-13.1	1.9	1114.4
$2p^3\ ^2P_{3/2}$	1463.4	- 5.1	-12.5	1.9	1447.6

Transition Parameters

The percentage of present *S* values for E1, E2, M1 and M2 transitions falling in each of the NIST accuracy class

	Percentage of Transitions			
Accuracy class	E1	E2	M1	M2
$A+$ ($\leq 2\%$)	80	61	98.8	85.7
A ($\leq 3\%$)	4	6	0.5	6
$B+$ ($\leq 7\%$)	6	19	0.5	6
B ($\leq 10\%$)	2	14	0.1	1
$C+$ ($\leq 18\%$)	3	0	0.1	1
C ($\leq 25\%$)	1	0	0	0.1
$D+$ ($\leq 44\%$)	2	0	0	0.1
D ($\leq 54\%$)	0	0	0	0
E ($> 54\%$)	1	0	0	0

Type	Number of transitions
E1	10562
E2	8568
M1	6000
M2	7224

Atomic-structure calculations for Ar-Like Kr^{18+} using MCDHF and MBPT methods

1. The lowest 150 fine-structure levels belonging to the $3s^23p^6$, $3s^23p^53d$, $3s3p^63d$, $3s^23p^43d^2$, $3s3p^53d^2$ configurations in Ar-like Kr^{18+} using GRASP2018 code.
2. Energy levels, lifetime, wavelength, weighted oscillator strength, transition probabilities and line strengths for electric and magnetic dipole (E1,M1) and quadrupole (E2,M2) transitions are calculated.
3. Since very limited measurements are available for comparison with the present results, we performed another set of calculations using many body perturbation theory (MBPT).

Methodology

Ar like Kr - $1s^2 2s^2 2p^6 3s^2 3p^6$

Multireference set -

Even	Odd
$3s^2 3p^6$	$3s^2 3p^5 3d^1$
$3s^1 3p^6 3d^1$	$3s^1 3p^5 3d^2$
$3s^2 3p^4 3d^2$	$3s^2 3p^3 3d^3$
$3s^1 3p^4 3d^3$	

$1s^2 2s^2 2p^6$: Inactive core

We performed these calculations in active set (AS) approach i.e., by adding orbitals layer by layer as follows,

AS{1} = {4s,4p,4d,4f}

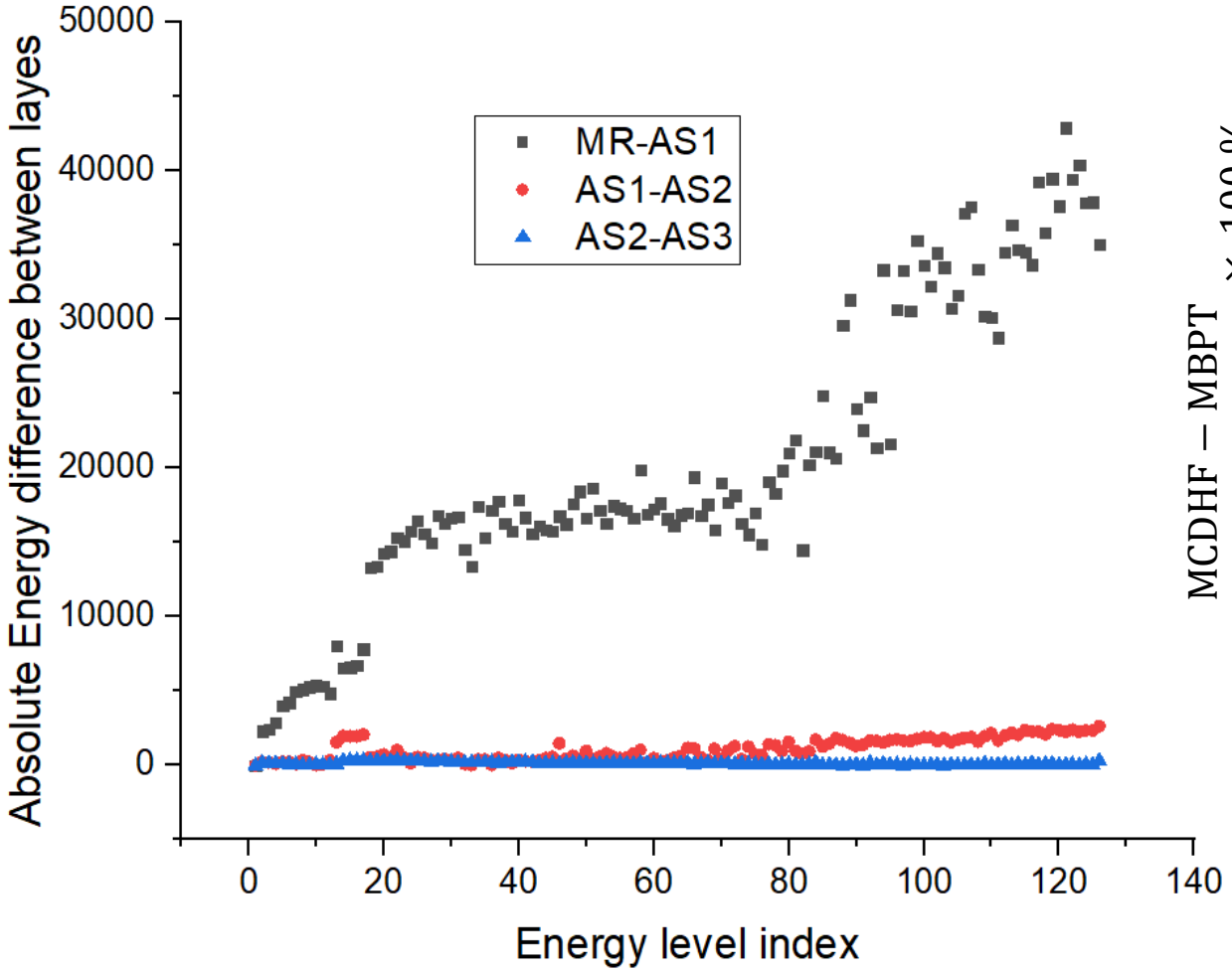
AS{2} = AS{1} + {5s,5p,5d,5f,5g}

AS{3} = AS{2} + {6s,6p,6d,6f,6g}

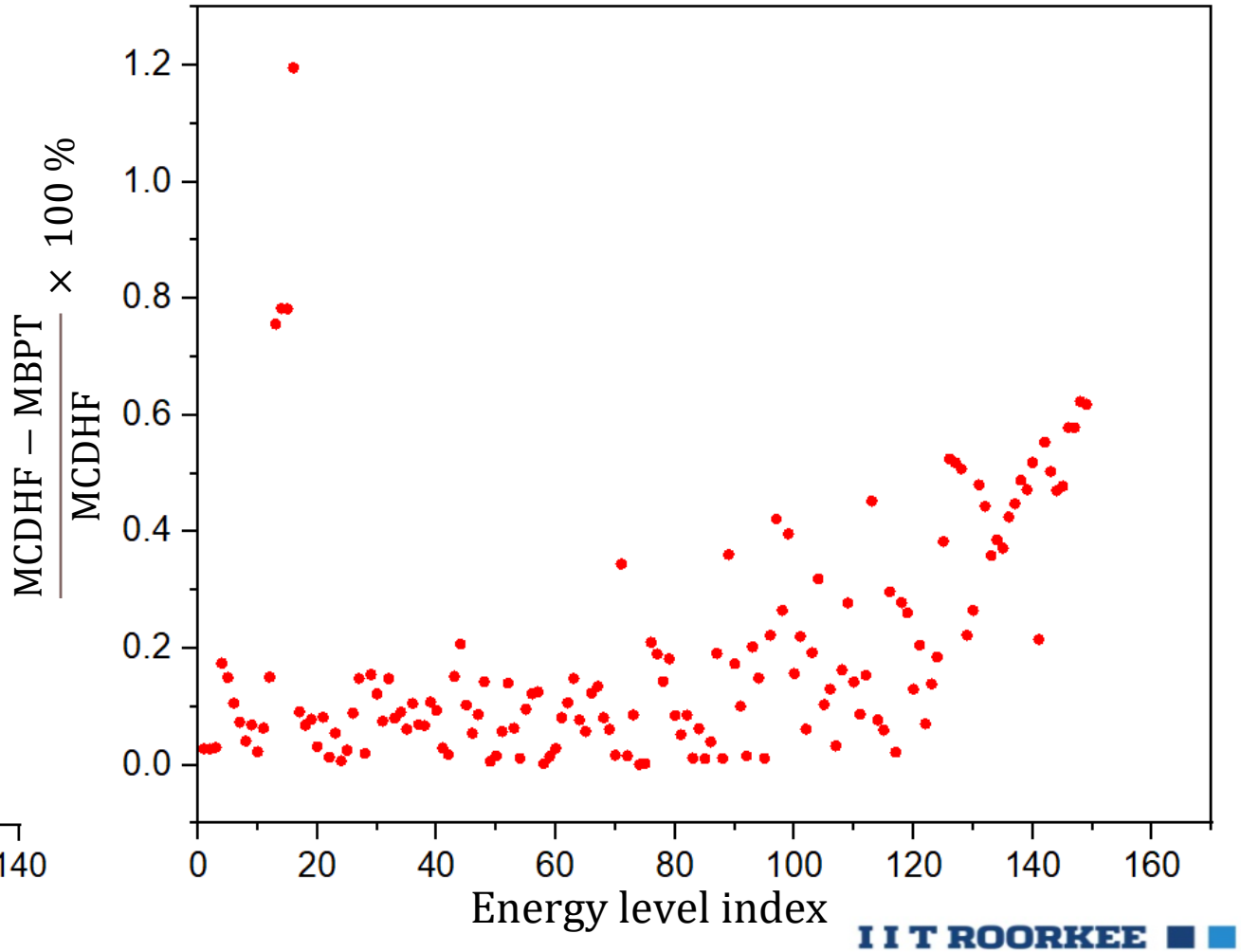
AS{4} = AS{3} + {7s,7p,7d,7f,7g}

Results

The convergence of present energies with increasing active layers



Comparison of MCDHF and MBPT energies



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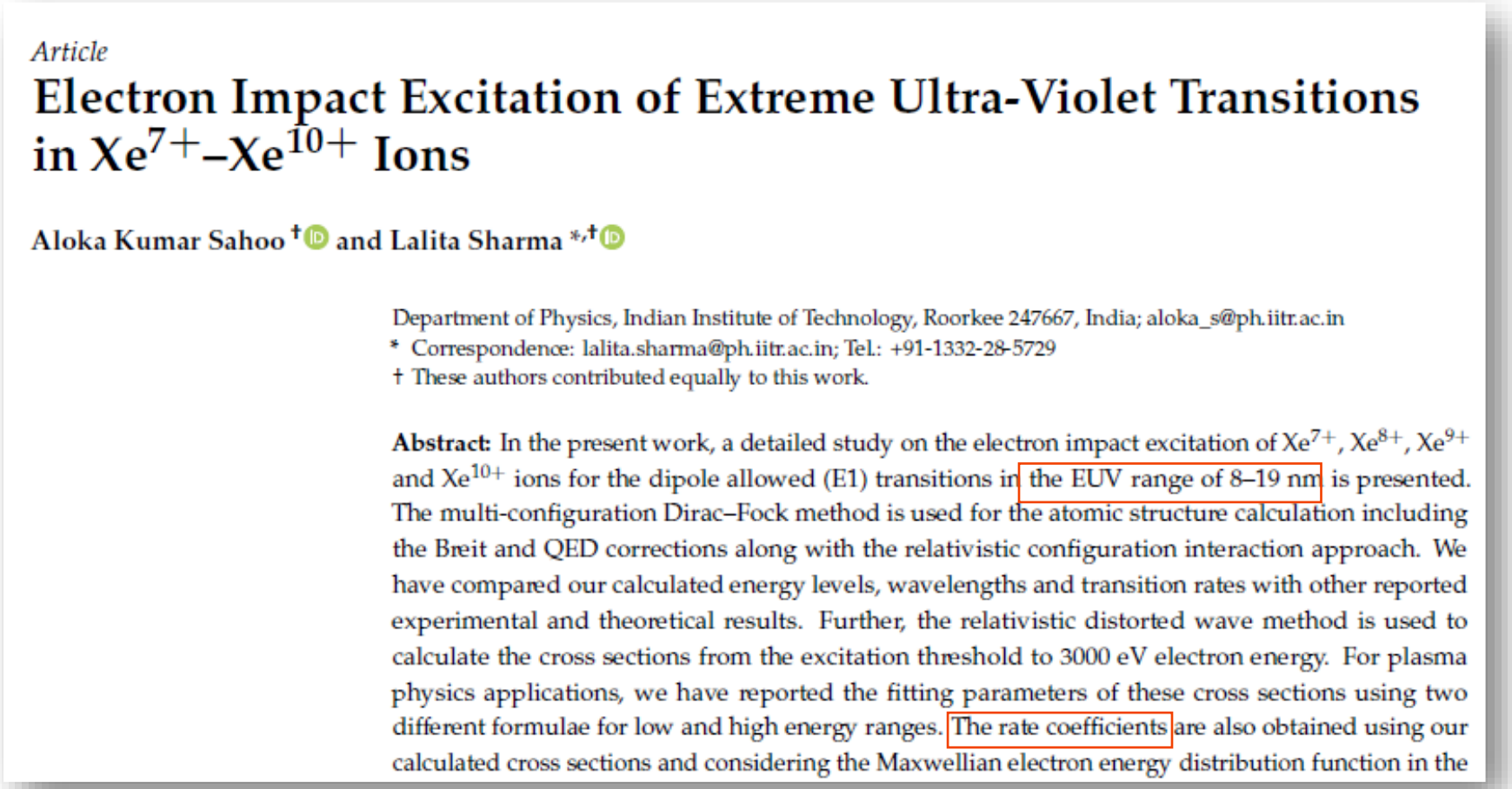

Article

Electron Impact Excitation of Extreme Ultra-Violet Transitions in Xe^{7+}–Xe^{10+} Ions

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Abstract: In the present work, a detailed study on the electron impact excitation of Xe^{7+}, Xe^{8+}, Xe^{9+} and Xe^{10+} ions for the dipole allowed (E1) transitions in the EUV range of 8–19 nm is presented. The multi-configuration Dirac–Fock method is used for the atomic structure calculation including the Breit and QED corrections along with the relativistic configuration interaction approach. We have compared our calculated energy levels, wavelengths and transition rates with other reported experimental and theoretical results. Further, the relativistic distorted wave method is used to calculate the cross sections from the excitation threshold to 3000 eV electron energy. For plasma physics applications, we have reported the fitting parameters of these cross sections using two different formulae for low and high energy ranges. The rate coefficients are also obtained using our calculated cross sections and considering the Maxwellian electron energy distribution function in the

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