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Atomic Data for Injected Impurities in Fusion Plasmas

Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

18 – 20 December 2024

Prepared by

C. Hill

December 2024

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Abstract

10 experts in the field of atomic collisional physics and edge-plasma modelling for magnetic confinement fusion devices, together with IAEA Staff, met at IAEA Headquarters in Vienna, Austria from 18 – 20 December 2024 for the Second Research Coordination Meeting of the IAEA Coordinated Research Project (CRP) F43026: *Atomic Data for Injected Impurities in Fusion Plasmas*. Workplans for the last 18 months of this project were reviewed, ongoing work discussed, collaborative activities planned, and data priorities set. The proceedings of the meeting are summarized in this report.

December 2024

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1. Introduction

The IAEA Coordinated Research Project (CRP) on *Atomic Data for Injected Impurities in Fusion Plasmas* ("Injected Impurities") is intended to provide evaluated and recommended data for the atomic processes relevant to the behaviour of first-row and noble gas atoms in edge and divertor plasmas for disruption mitigation and diagnostics. This report summarizes the second RCM, held at IAEA Headquarters from 18 – 20 December 2024. More information about the background and the objectives of the project can be found on the AMD Unit's website at https://amdis.iaea.org/CRP/injected-impurities.

There were 10 research groups represented in the meeting, from nine Member States of the IAEA. The proceedings of the meeting are summarized in Section 2 and the discussions in Section 3. Workplan reviews from each participating group are provided in Section 4. The list of participants is in Appendix 1 and the meeting agenda is given in Appendix 2. Summary abstracts of presentations are presented in Appendix 3.

2. Proceedings

The meeting was opened by the Head of the Nuclear Data Section, A. Koning and staff of the Atomic and Molecular Data Unit, C. Hill and K. Heinola. After a brief introduction from the participants, the CRP goals and meeting objectives were reviewed. Participants presented their research activities during the first period of the CRP in the first half of the meeting (Section 3 and Appendix 3 of this report), which was followed by discussion sessions focused on methodologies and priorities for the calculation of missing data relevant to injected impurity modelling (Section 4). Two code-comparison activities (Section 5) were planned:

(1) to calculate the atomic structure and radiative characteristics of low-charge states of argon particularly relevant to the relatively low plasma temperatures of the edge-regions of magnetic confinement fusion devices where argon is deliberately injected as an impurity to improve core plasma confinement; and:

(2) to validate computational methods and model potentials for calculating charge exchange cross sections, with a focus on collisions between hydrogen isotope atoms and ions and various charge states of neon and argon.

3. Work Plan Summaries

Connor BALLANCE, Queen's University Belfast (QUB), UK

Electron-impact excitation for doubly ionised Tungsten [1] has been compared with observations taken at the CTH (Compact Toroidal Hybrid) experiment at Auburn University. Synthetic spectra as a result of Collisional Radiative (CR) modelling reveals good agreement with strong line identification of Lawson et al [2] and simple line ratios suggests lines that may offer temperature and density diagnostics.

Three new atomic structure and electron-impact scattering models have been developed and compared in order to better constrain the differences in the atomic data for Ar^{+} and how they impact well-known plasma diagnostics [3].

Publications

[1] M McCann *et al., J. Phys. B: At. Mol. Opt. Phys.* **57** 235202 (2024)
[2] K Lawson *et al., Phys. Scr.* **97** (2022) 055605: https://doi.org/10.1088/1402-4896/ac5eff
[3] McElroy, N. E., Ramsbottom, C. A., Ballance, C. P., Badnell, N. R., O'Mullane, M. G., Loch, S. D., E. N. Williamson, "Atomic structure, electron-impact excitation and collisional-radiative modelling for Ar II", *Journal of Quantitative Spectroscopy & Radiative Transfer* **325**, 109080 (2024): https://doi.org/10.1016/j.jqsrt.2024.109080

Haikel JELASSI, National Center of Nuclear Sciences and Technologies (CNSTN), Tunisia

Ab-initio MCDHF/RCI calculations of mass- and field shifts isotopes parameters of the $1s^2\ ^1S_0 - 1s\ 2p\ ^1P^o_1$ and $1s^2\ ^1S_0 - 1s\ 2p\ ^3P^o_{0,1,2}$ transitions in He-like ions for the sequence $2 \leq Z \leq 83$

Based on the multiconfiguration Dirac-Hartree-Fock method, the field shift and mass shift parameters of the $1s^2\ ^1S_0 - 1s\ 2p\ ^1P^o_1$ and $1s^2\ ^1S_0 - 1s\ 2p\ ^3P^o_{0,1,2}$ transitions in He-like ions for the sequence $2 \leq Z \leq 83$ are calculated with high precision. The total value of the isotope shift is determined by the sum of the mass- and field-shifts. With the inclusion of the Breit interaction and the leading QED corrections, we find that the mass shift parameters of these transitions do not change monotonously along the isoelectronic sequence in the high-*Z* range due to the relativistic nuclear recoil effects. In addition, the field shifts and mass shifts of these four transitions are estimated and compared along the isoelectronic sequence. This work has been published in the Journal of Quantitative Spectroscopy and Radiative Transfer**.**

Extensive Atomic Structure Calculations and Study of Plasma Parameters using Line Intensity Ratios for the Spectra Ne VIII, Fe XXIV and Kr XXXIV in The Lithium Isoelectronic Sequence

Extensive and accurate computations have been conducted on the energy levels, wavelengths, weighted oscillator strengths, transition rates, line intensity ratios and plasma parameters for the lowest 35 odd and even parity states arising from the $1s^2\ nl$ ($n = 1 - 6$, $0 \leq l \leq n - 1$) configurations of lithium-like neon, iron, and krypton. These calculations involved the Multiconfigurational Dirac-Hartree-Fock (MCDHF) method followed by the Relativistic Configuration Interaction (RCI) approach. Transition rates were also determined for electric-multipole (dipole (E1), quadrupole (E2)) and magnetic-multipole (dipole (M1), quadrupole (M2)). The calculations incorporated Breit interactions and quantum electrodynamics effects (QED) as perturbations within the extensive relativistic configuration interaction (RCI) approach. Our results were compared with other existing theories in the literature and the data from the NIST database revealing a significant level of agreement. Additionally, the line intensity ratios and plasma parameters specifically, plasma temperature and electron density were determined. Almost all atomic data of Li-like ions presented in this work were calculated for the first time especially those for Fe XXIV and Kr XXXIV. This interesting work has been accepted for publication in the journal *Zeitschrift für Naturforschung A.*

Accurate and complete MCDHF calculations of atomic data for In XLVIII

Energy levels, wavelengths, weighted oscillator strengths, transition probabilities and lifetimes are calculated for all levels of $1s^2$ and $1snl$ ($n = 2 - 6$) configurations of He-like indium ion (In XLV III). The calculations were carried out using the GRASP2018 code in order to provide theoretically the most accurate data. Transition probabilities are reported for all the E1, E2, M1 and M2 transitions. Breit interactions and quantum electrodynamics effects are included in the RCI calculations. Comparisons were made with other calculations and a good agreement was found which confirms the reliability of our results. We were presenting some new and missing data for the He-like indium in this work for the first time.

Publications

Ab-initio MCDHF/RCI calculations of mass- and field shifts isotopes parameters of the $1s^2\ ^1S_0 - 1s\ 2p\ ^1P^o_1$ and $1s^2\ ^1S_0 - 1s\ 2p\ ^3P^o_{0,1,2}$ transitions in He-like ions for the sequence, S. B. Nasr, S. Manai, D. E. Salhi, H. Jelassi, *Journal of Quantitative Spectroscopy and Radiative Transfer* **315**, 108890 (2024): https://doi.org/10.1016/j.jqsrt.2023.108890.

Extensive Atomic Structure Calculations and Study of Plasma Parameters using Line Intensity Ratios for the Spectra Ne VIII, Fe XXIV and Kr XXXIV in The Lithium Isoelectronic Sequence, S. Manai, D. E. Salhi, H. Jelassi, *Zeitschrift für Naturforschung A*, accepted.

Accurate and complete MCDHF calculations of atomic data for In XLV III, submitted to *Journal of the Korean Physical Society*.

Valdas JONAUSKAS, Institute of Theoretical Physics and Astronomy, Vilnius University, Lithuania

Single ionization processes in Ne^{2+}, Ne^{3+}, and Ne^{4+} ions were analyzed using the distorted wave (DW) approximation, implemented in the Flexible Atomic Code (FAC). Cross sections were studied for the energy levels of the ground configurations of these ions. Convergence of the EA channels is estimated by analyzing excitations up to shells with the principal quantum numbers $n \leq 20$. A good agreement with experimental data is obtained for the single ionization cross sections.

Publications

V. Jonauskas, Electron-impact single ionization for N^+ ion, *Mon. Not. R. Astron. Soc.* **526**, 2104 (2023). DOI: 10.1093/mnras/stad2893

A. Kynienė, Š. Masys, V. Jonauskas, Electron-impact single ionization for the N^{2+} and N^{3+} ions, *J. Quant. Spectrosc. Radiat. Transf.* **315**, 108898 (2024). DOI: 10.1016/j.jqsrt.2024.108898

A. Kynienė, Š. Masys, V. Jonauskas, Electron-impact ionization for Ne^{3+} and Ne^{4+}, *J. Quant. Spectrosc. Radiat. Transf.* **330**, 109224 (2025). DOI: 10.1016/j.jqsrt.2024.109224

Alisher KADYROV, Faculty of Science and Engineering, Curtin University, Australia

Within the CRP on Atomic Data for Injected Impurities in Fusion Plasmas, we have so far calculated

1. The total ionisation cross section and the total and n-resolved charge-exchange and target-excitation cross sections in partially stripped C^{2+} and C^{3+} ion collisions with ground-state atomic hydrogen. Calculations have been performed using the two-centre wave-packet convergent close-coupling approach across a broad projectile energy range from 1 keV/u to 1 MeV/u.

2. State-selective charge exchange in collisions of Ar^{16+} ions with ground-state hydrogen atoms has been modelled using the two-centre wave-packet convergent close-coupling approach. The n-resolved electron-capture cross sections have been presented for capture into states with n = 6− 19, where n is the final-state principal quantum number. The most important of these are the cross sections for capture into the n = 14− 17 states, which are used in charge-exchange recombination spectroscopy techniques.

3. Singly and doubly differential cross sections for ionisation in p and He^{2+} collisions with H, He and H_2.

Publications

M. Charlton, H. B. Ambalampitiya, I. I. Fabrikant, I. Kalinkin, D. V. Fursa, A. S. Kadyrov, and I. Bray, Antiproton collisions with excited positronium, *Phys. Rev. A* **107**, 012814 (2023).

C. T. Plowman, I. B. Abdurakhmanov, I. Bray, and A. S. Kadyrov, Energy and angular distributions of electrons emitted in proton collisions with molecular hydrogen, *Phys. Rev. A* **107**, 032824 (2023).

K. H. Spicer, C. T. Plowman, S. U. Alladustov, I. B. Abdurakhmanov, I. Bray, and A. S. Kadyrov, Doubly differential cross sections for ionisation in proton-helium collisions at intermediate energies: Energy and angular distribution of emitted electrons, *Eur. Phys. J. D* **77**, 131 (2023).

A. M. Kotian, C. T. Plowman, and A. S. Kadyrov, Electron capture and ionisation in He^{2+} collisions with H_2, *Eur. Phys. J. D* **77**, 163 (2023).

K. H. Spicer, C. T. Plowman, M. Schulz, and A. S. Kadyrov, Doubly differential ionization in proton-helium collisions at intermediate energies: Energy distribution of emitted electrons as a function of scattered-projectile angle, *Phys. Rev. A* **108**, 022803 (2023).

C. T. Plowman, K. H. Spicer, and A. S. Kadyrov, Calculation of energy and angular distributions of electrons produced in intermediate-energy p+H_2 collisions, *Atoms* **11**, 112 (2023).

H. B. Ambalampitiya, J. Stallbaumer, I. I. Fabrikant, I. Kalinkin, D. V. Fursa, A. S. Kadyrov, and I. Bray, Near-threshold collisional dynamics in the e − e+p system, *Phys. Rev. A* **108**, 032808 (2023).

C. Hill, Dipti, K. Heinola, A. Dubois, N. Sisourat, A. Taoutioui, H. Agueny, K. Tőkési, I. Ziaeian, C. Illescas, A. Jorge, L. Méndez, A. Kadyrov, N. Antonio, A. Kotian, T. Kirchner, A. Leung, J. Ko, J. Lee, O. Marchuk, M. O'Mullane, E. Litherland-Smith, G. Pokol, O. Asztalos, P. Balazs, Y. Wu, C. Jia, L. Liu, and J. Wang, Atomic collisional data for neutral beam modeling in fusion plasmas, *Nucl. Fusion* **63**, 125001 (2023).

I. Bray, I. Kalinkin, D. V. Fursa, A. S. Kadyrov, H. B. Ambalampitiya, and I. I. Fabrikant, Positron-hydrogen scattering: internal consistency and threshold behaviour for excited states, *Eur. Phys. J. D* **77**, 194 (2023).

C. T. Plowman, K. H. Spicer, M. Schulz, and A. S. Kadyrov, Scattering-angle dependence of doubly differential cross sections for ionization in proton collisions with molecular hydrogen, *Phys. Rev. A* **108**, 052809 (2023).

N. W. Antonio, C. T. Plowman, I. B. Abdurakhmanov, and A. S. Kadyrov, Calculations of the integrated cross sections in dressed carbon-ion collisions with atomic hydrogen, *Phys. Rev. A* **109**, 012817 (2024).

S. U. Alladustov, C. T. Plowman, M. S. Schöffler, I. Bray, and A. S. Kadyrov, Singly differential studies of one-electron processes in He^{2+} − He collisions, *Phys. Rev. A* **109**, 022805 (2024).

K. H. Spicer, C. T. Plowman, N. W. Antonio, M. S. Schöffler,, M. Schulz, and A. S. Kadyrov, Ruling out a saddle-point mechanism of ionization in intermediate-energy ion-atom collisions, *Phys. Rev. A* **109**, 062805 (2024).

C. T. Plowman, K. H. Spicer, N. W. Antonio, M. S. Schöffler,, M. Schulz, I. Bray, and A. S. Kadyrov, Doubly differential cross sections for ionization in proton collisions with atomic hydrogen: Energy and angular distribution of emitted electrons, *Phys. Rev. A* **110**, 022804 (2024).

A. M. Kotian, N. W. Antonio, O. Marchuk, and A. S. Kadyrov, State-selective electron capture in Ar^{16+} + H(1s) collisions for charge-exchange recombination spectroscopy, *Plasma Phys. Control. Fusion* **66**, 095014 (2024).

N. W. Antonio, I. Bray, and A. S. Kadyrov, Unified treatment of atomic excitation and ionization, *Phys. Rev. A* **110**, 032810 (2024).

N. W. Antonio, I. Bray, and A. S. Kadyrov, Connecting excitation and ionization cross sections in electron-atom scattering, *Phys. Rev. A* **110**, 062810 (2024).

I. B. Abdurakhmanov, N. W. Antonio, M. Cytowski, and A. S. Kadyrov, Portable GPU implementation of the WP-CCC ion-atom collisions code, in High Performance Computing, edited by M. Weiland, S. Neuwirth, C. Kruse, and T. Weinzierl (Springer Nature Switzerland, Cham, 2025) pp. 102–114.

Xinwen MA, Institute of Modern Physics (IMP), Chinese Academy of Sciences (CAS), China

During the first part of the CRP, experimental studies of charge exchange in ion-atom collisions and dielectronic recombination rate coefficient were conducted using ions from accelerators. The measurements include:

1. Charge exchange interactions between highly charged ions and atomic helium, neon, and molecular hydrogen were investigated, with collision energies ranging from approximately 2 keV/u to 100 keV/u. Differential charge exchange cross sections were obtained, resolved by principal quantum numbers and angular momentum quantum numbers. The experimental data were compared with various theoretical models. It was clearly demonstrated that all classical models previously used to evaluate angular momentum number distributions (*l*-distribution) are inadequate; these models fail to accurately describe the *l*-distribution and do not properly account for the collision energy dependence, even in the low energy range. In contrast, quantum theory-based models, including AOCC and ASCC, can accurately describe the *l*-distributions, although they require significantly

greater computational power. Notably, by directly measuring the cross-section ratio of triplet to singlet states in single electron capture involving C^{3+} ions colliding with helium, we confirmed that the statistical assumptions commonly applied in many contexts do not hold.

The measured charge exchange cross-sections, differential in principal quantum numbers *n* and angular momentum numbers *l*, include the following collision systems: C^{3+} + He, C^{4+} + He, O^{4+} + He, O^{6+} + He/H_2/Ne, Ne^{7+} + He/H_2, S^{q+}(q = 11–15) + He/H_2. (Publications 1-7).

2. Dielectronic recombination rate coefficient has been measured for Kr^{25+} and Kr^{35+} ions. The corresponding DR resonance energies and strengths have been calculated by using the flexible atomic code (FAC) and AUTOSTRUCTURE to understand the measured results. In particular, the resonances from the trielectronic recombination due to $2s^22p^2+e^- \rightarrow 2p^4[^1D^2]6l$ have been identified with the help of the FAC calculation. Temperature-dependent plasma recombination rate coefficients were derived from the measured DR rate coefficients for the temperature range 10^3 – 10^7 K and compared with our FAC calculations as well as the previous AUTOSTRUCTURE calculations. In addition, the plasma recombination rate coefficients for $Ar^{12+, 14+}$, $Ca^{14+, 16+, 17+}$, Ni^{19+}, and Kr^{25+} ions are summarized. The present work provides the benchmark data for astrophysical and laboratory plasma modeling.

   The derived plasma rate coefficients are in good agreement with the FAC and AUTOSTRUCTURE calculations (Publications 8-10).

Publications

1. Xiaolong Zhu, Shaofeng Zhang, Yong Gao, Dalong Guo, Jiawei Xu, Ruitian Zhang, Dongmei Zhao, Kaizhao Lin, Xubin Zhu, Dadi Xing, Shucheng Cui, Stylianos Passalidis, Alain Dubois and X. Ma, Direct Evidence of Breakdown of Spin Statistics in Ion-Atom Charge Exchange Collisions, Phys. Rev. Lett. 133, 173002 (2024): https://doi.org/10.1103/PhysRevLett.133.173002
2. K. Z. Lin, Y. Gao, X. L. Zhu, S. F. Zhang, T. Cao, D. L. Guo, X. Shan, D. M. Zhao, X. J. Chen, and X. Ma, Subshell-resolved electron capture in O^{4+}-He collisions near Bohr velocity, Phys. Rev. A **109**, 052811 (2024): https://doi.org/10.1103/PhysRevA.109.052811
3. X B Zhu, D D Xing, K Z Lin, S C Cui, X L Zhu, Y Gao, D L Guo, D M Zhao, S F Zhang and X Ma, Study of state-selective single-electron capture in slow Ne^{7+} colliding with He and H_2 target, J. Phys. B: At. Mol. Opt. Phys. **57**, 045001 (2024): https://doi.org/10.1088/1361-6455/ad2547
4. Xiaolong Zhu, Shucheng Cui, Dadi Xing, Jiawei Xu, B. Najjari, Dongmei Zhao, Dalong Guo, Yong Gao, Ruitian Zhang, Maogen Su, Shaofeng Zhang, and Xinwen Ma, State-selective charge exchange cross sections in collisions of highly-charged sulfur ions with helium and molecular hydrogen, Chin. Phys. B **33**, 023401 (2024). https://doi.org/10.1088/1674-1056/ad0b01
5. Shucheng Cui, Dadi Xing, Xiaolong Zhu, Maogen Su, Yong Gao, Dalong Guo, Dongmei Zhao, Shaofeng Zhang, Yanbiao Fu and Xinwen Ma, n-resolved single-electron capture in slow O^{6+}-Ne collisions, *Chinese Phys. B* 33 073401 (2024): 10.1088/1674-1056/ad39d2
6. T. Cao, T. Meng, Y. Gao, S. F. Zhang, R. T. Zhang, S. Yan, X. L. Zhu, J. Wang, P. Ma, B. Ren, Z. H. Xia, D. L. Guo, C. J. Zhang, K. Z. Lin, S. Xu, B. Wei, **X. Ma**, State-selective Charge Exchange in 19.5–100 keV amu^{-1} O^{6+} Collision with He and H_2, The Astrophysical Journal Supplement Series 266 (2023) 20: https://iopscience.iop.org/article/10.3847/1538-4365/accba2
7. D. L. Guo, R. T. Zhang, X. L. Zhu, Y. Gao, D. M. Zhao, K. Z. Lin, X. B. Zhu, S. F. Zhang, and **X. Ma**, Production of autoionizing states by double-electron capture in intermediate-energy C^{4+} + He collisions, Phys. Rev. A 107, 012801 (2023): https://link.aps.org/doi/10.1103/PhysRevA.107.012801
8. Zhongkui Huang, Shuxing Wang, Weiqiang Wen, Hanbing Wang, Wanlu Ma, Chongyang Chen, Chunyu Zhang, Dongyang Chen, Houke Huang, Lin Shao, Xin Liu, Xiaopeng Zhou, Lijun Mao, Jie Li, Xiaoming Ma, Meitang Tang, Jiancheng Yang, Youjin Yuan, Shaofeng Zhang, Linfan Zhu, and **Xinwen Ma**, Absolute dielectronic recombination rate coefficients of highly charged ions at the storage ring CSRm and CSRe, Chinese Physics B 32, 073401 (2023): https://iopscience.iop.org/article/10.1088/1674-1056/acbc69

9. Wan-Lu Ma, Shu-Xing Wang, Zhongkui Huang, Weiqiang WEN, Hanbing Wang, Dong-Yang Chen, Xin Liu, Xiao-Peng Zhou, Hou-Ke Huang, Lin Shao, Chang Liu, Chunyu Zhang, Chongyang Chen, Lijun Mao, Xiaoming Ma, Jie Li, Mei-Tang Tang, Kai-Ming Yan, Yun-Bin Zhou, Dongmei Zhao, Youjin Yuan, Jiancheng Yang, **Xinwen Ma**, and Lin-Fan Zhu, Dielectronic recombination rate coefficients of carbon-like Kr^{30+}, Journal of Physics B: Atomic, Molecular and Optical Physics, 56 095203 (2023): https://iopscience.iop.org/article/10.1088/1361-6455/acc49d
10. C. Y. Zhang, B. S. Yan, K. Wang, R. Si, K. Yao, W. L. Ma, Z. K. Huang, W. Q. Wen, X. W. Ma, L. F. Zhu, C. Y. Chen, and N. R. Badnell, Benchmarking Dielectronic Recombination Rate Coefficients for Carbon-like Ca^{14+}, The Astrophysical Journal, 976:84 (11pp), 2024 November 20: https://doi.org/10.3847/1538-4357/ad812b

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During the first part of the CRP, and according to the plan of activities proposed, total and state-selective charge exchange cross sections for Ar^{18+} and Ne^{10+} collisions on H(1s) and H*(n=2) were calculated using three variants of the classical trajectory Monte Carlo method (CTMC, E-CTMC and Z-CTMC). The underlying idea was to determine which of these models provided the best agreement with the reported experimental data and the theoretical data available from state-of-the art quantum mechanical methods. The study performed for H(1s) concluded that the Z-CTMC method provided the best overall agreement with these data. This study has been recently submitted for publication [1].
Meanwhile, the calculation of charge exchange cross sections for H*(n=2) is actually in its final stage and the analysis is expected to be submitted for publication during the first quarter of 2025.

[1] N. D. Cariatore, N. Bachi, E. Acebal, S. Otranto, "State-selective electron capture in bare Ne and Ar collisions with H(1s): A critical analysis of classical trajectory methods of relevance for charge-exchange recombination spectroscopy", *Plasma Physics and Controlled Fusion* (submitted 2024)

Yuri RALCHENKO, National Institute of Standards and Technology, United States of America

Over the last 18 months, NIST activities related to this CRP included:
- Release of two new versions of the Atomic Spectra Database with extensively updated data on Li-like and He-like ions across a very large range of elements: http://physics.nist.gov/asd;
- Addition of the online generation of Ritz wavelengths; this would increase the number of spectral lines for N, Ne, Ar and Xe by a factor of 5-7;
- Collisional-radiative modelling of Ne EUV spectra from the NIST Electron Beam Ion Trap; this modelling is shown to provide direct connection to simulations of Maxwellian plasmas in magnetic fusion devices (to be published);
- Measurement and collisional-radiative analysis of Knn' dielectronic resonances in Li-like Ar^{16+}; these resonances are highly important for diagnostics of magnetic fusion plasmas (to be published).

Lalita SHARMA, Indian Institute of Technology, Roorkee, India

Details of calculations

1. CR Model of Kr III plasma

A collisional radiative model for Kr III in the ultraviolet regime is developed. For this purpose, atomic parameters for $4s^24p^4$, $4s4p^5$, $4s^24p^3nl$, and $4s^24p^35d$ configurations with n ranging from 5 to 7 and l = s, p, using the multiconfiguration Dirac-Hartree-Fock method are calculated. The effects of Breit and radiative quantum electrodynamic corrections are also included. Electron impact excitation cross-sections from the ground state, along with four metastable states arising from the $4s^24p^4$ configuration to all fine structure levels of interest, are calculated using the relativistic distorted wave method. The reliability of the model is tested by comparing the predicted results with the previous measurements. The detailed results are available at S. Rathi and L. Sharma, "A Collisional-Radiative Model for Kr III Ions", *Atoms* **12**(8), 39 (2024): https://doi.org/10.3390/atoms12080039.

2. CR Model of Kr^{+} plasma

An extensive spectroscopic investigation of Kr^{+} plasma has been carried out through a comprehensive collisional-radiative plasma model along with the calculations of electron impact excitation cross-sections. The fully relativistic distorted wave method has been employed to calculate the detailed electron impact cross-sections for the transitions from the ground state, four metastable states of $4p^4 4d$ and a quasi-metastable state of $4p^4 5s$ to the fine structure levels of $4p^4\ ns (7 \leq n \leq 9)$, $4p^4 np$, $4p^4 nd\ (6 \leq n \leq 9)$ and $4p^4\ nf\ (4 \leq n \leq 9)$ excited states. For this purpose, the relativistic multi-configuration Dirac-Fock method is applied to compute the Kr^{+} ionic structure, Kr^{+} ion bound-state wave functions, excitation energies, oscillator strengths and transition probabilities. These results are compared with the previously reported values. Further, the complete set of electron impact excitation cross-sections has been incorporated in the collisional-radiative model along with the other relevant kinetic processes, viz. electron impact ionization, de-excitation, three-body recombination, and radiative decay. To validate the reliability of the electron collision data and the present collision radiative model, the measurements of Mar et al [J. Phys. B: At. Mol. Opt. Phys. 393,709 (2006)] at 40 μs and 90 μs instants of plasma lifetime have been utilized for the diagnosis of experimentally measured pulsed discharge Kr^{+} plasma at 3.3×10^3 Pa. The measured line emissions from Kr^{+} in the wavelength range of 457 – 485 nm are compared with the intensities obtained from the present theoretical collision radiative model to obtain the plasma parameters such as electron temperature (T_e) and electron density (n_e). The electron temperature results at 40 μs and 90 μs reported by Mar *et al.* obtained through the Boltzmann plots, have been compared with the values obtained from the present collision radiative model. The published paper and results can be accessed from https://doi.org/10.1016/j.sab.2024.106953

3. Ar-like Kr^{18+}

In this study, we present a detailed analysis of atomic properties for Kr XIX, specifically focusing on the lowest 128 fine-structure levels originating from the $3s^2 3p^6$, $3s^2\ 3p^5 3d$, $3s3p^6 3d$ and $3s^2\ 3p^4 3d^2$ configurations. We report energy levels, lifetimes, wavelengths, weighted oscillator strengths, and transition probabilities for multipole transition types (E1, E2, M1, and M2). To achieve this, we employed the GRASP2018 code, which implements the fully relativistic multiconfigurational Dirac–Hartree–Fock method and accounts for Breit interaction and quantum electrodynamic effects. We performed another set of calculations using the many-body perturbation theory implemented in the flexible atomic code (FAC). By comparing the results obtained from GRASP2018 and FAC, we established the accuracy and consistency of our calculations. Furthermore, using the relativistic distorted wave theory, we studied electron impact excitation of all transitions to upper levels from the ground and metastable levels and reported excitation cross sections for incident electron energies up to 5 keV. To enhance the practical utility of our findings, we also provided analytical fittings of these cross sections and excitation rate coefficients for their applications in plasma modeling. This work contributes to the atomic properties and excitation cross sections of Kr XIX, addressing a marked gap in the available atomic data. Details can be seen from our published paper at https://doi.org/10.1016/j.jqsrt.2024.109012.

4. S-like Xe^{38+}

Atomic structure parameters for levels corresponding to $2s^2 2p^6 3s^2 3p^4$, $2s^2 2p^6 3s 3p^5$, $2s^2 2p^6 3s^2 3p^2\ 3d^2$, $2s^2 2p^6 3s 3p^4 3d$ and $2s^2 2p^6 3s^2 3p^3 3d$ configurations of S-like Xe^{38+} are calculated using the fully relativistic multiconfiguration Dirac-Hatree-Fock method followed by the subsequent relativistic configuration interaction (RCI) calculations. The parameters evaluated include energies of the lowest 75 levels and E1, M1, E2, and M2 transition parameters among these levels. The effect of the choice of virtual orbitals for generating the wavefunctions is discussed. The accuracy of our line strengths is established through the rigorous calculations of their associated uncertainties using three different methods. Another set of calculations using the many-body perturbation theory (MBPT) to validate the present MCDHF-RCI energies is carried out. Further, the electron impact excitation cross-sections using the relativistic distorted wave theory are determined for all transitions from the ground and metastable states in the incident electron energy range from the excitation threshold to 10 keV. For plasma physics applications, the fitting parameters for these cross sections employing two distinct equations tailored for low and high-energy regimes are reported. Moreover, the rate coefficients are determined in the electron temperatures range of 15 eV to 100 eV by taking into account the Maxwellian electron energy distribution function and our computed cross-sections. In addition to addressing the atomic data gap in highly charged Xe ions, the present results are of good accuracy and can serve as benchmark tests for other theoretical evaluations. Moreover, they can also assist in line identification of the complex spectra of highly charged sulphur-like xenon ions. Results are available in our paper https://doi.org/10.1016/j.sab.2024.106897.

Publications

1. S. Rathi and L. Sharma, "A Collisional-Radiative Model for Kr III Ions", *Atoms* **12**, 39 (2024): https://doi.org/10.3390/atoms12080039

2. A. Agrawal, S. Gupta, L. Sharma and R. Srivastava, "Spectroscopic study of Kr^{+} plasma through a detailed collisional radiative plasma model with extended ground, metastable and quasi-metastable electron impact excitation cross" *Spectrochimica Acta Part B: Atomic Spectroscopy*, **217** 106953 (2024): https://doi.org/10.1016/j.sab.2024.106953

3. N. Ghosh and L. Sharma, "Relativistic calculations of energy levels, lifetimes, transition parameters, and electron impact excitation cross sections for Kr XIX", *Journal of Quantitative Spectroscopy and Radiative Transfer* **322**, 109012 (2024): https://doi.org/10.1016/j.jqsrt.2024.109012

4. S. Rathi and L. Sharma, "Benchmarking calculations of level energies, transition parameters and electron impact excitation cross sections of S-like Xe^{38+}", *Spectrochimica Acta Part B: Atomic Spectroscopy* **214** 106897 (2024): https://doi.org/10.1016/j.sab.2024.106897

Nicolas SISOURAT, Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France

We have investigated the electron capture processes between N^{4+} and H, and N^{3+} and H. Results of the first collisional system are published in Phys. Rev. A and the corresponding data will be uploaded to CollisionDB. We are currently analyzing the results of the second system.

Publications

C. C. Jia, Y. Y. Qi, J. J. Niu, Y. Wu, J. G. Wang, A. Dubois, N. Sisourat, J. W. Gao, "Electronic processes in collisions between nitrogen ions and hydrogen atoms", *Phys. Rev. A* **110**, 062820 (2024).

Károly TŐKÉSI, HUN-REN Institute for Nuclear Research (ATOMKI)

We have calculated the charge exchange and ionization cross sections in collisions between Li^{+} ions on helium and nitrogen targets using the three-body Classical Trajectory Monte Carlo (CTMC) method [1]. The collision problem has been treated within the single active electron approximation. Our CTMC results for the capture process show good agreement with the existing results in the high projectile impact velocity range for both systems. In the low-impact velocity range, in the case of nitrogen targets, our CTMC results slightly overestimate the total cross sections of the capture process compared with the experimental data. However, the total capture cross section in the case of the helium target follows the trend of the experimental data even at low impact velocities. In addition, we presented and discussed the total ionization cross-sections of helium and nitrogen atomic targets with singly charged lithium ions.

We have presented a theoretical study of the ionization of nitrogen atom by a singly charged sodium ion using a classical treatment of the collision system [2]. Our work was a gap-filling work, as there are either very limited total cross section data are available or no available differential cross section data for this system. In our investigations, the Na^+-N collision system was reduced to a three-body problem. The interaction between the collision partners was described by the Garvey-type model potential. The total cross sections were presented in the impact energy range between 10 keV and 10 MeV and compared them with the available experimental data. The single and double differential cross sections are presented at 30, 40, 50 and 60 keV energies related to the energies of the plasma diagnostic used in the nuclear fusion. These impact energies of the differential cross section ensure that Na+ projectile can penetrate the plasma to a suitable depth, higher energies will reduce the interaction probability with the plasma components, while lower impact energy means low penetration distance in the plasma. We have shown that the maximum total ionisation cross section occurs at impact energy around 2000 keV. Moreover, we also showed that the majority of electrons are ejected at lower angles and in back scattering, furthermore, most of the ejected electrons have kinetic energy around 20 eV and below. The results provide a valuable tool for understanding the dynamics of ion-atom collisions and their applications in fusion plasma research. The study also highlights the usage of neutral alkali beams in diagnosing magnetically confined plasmas in the scrape-off layer and the edge.

We have presented the total (TCS) and differential (DCS) cross sections of the inter action of protons H^+ with neutral noble gases [3]. We used the three-body CTMC calculations based on Garvey-type model potential. In the model potential, only one active electron was included in the interaction dynamics, while the remaining electrons contributed to the screening effect. The TCSs of single-electron capture and single-electron ionization from different sub-shells were presented and discussed for the 0.2 keV – 50 MeV energy range. The ionization DCSs were presented and discussed for impact energy of 35 keV, focusing only on the outer sub-shells of the targets. Our results showed that the inner sub shells' contribution to the overall cross section is insignificant for low impact energies; however, when increasing the impact energies, the inner shells slowly start to contribute to the overall cross section. Our CTMC results of TCS of the ionization and electron-capture channels show very good agreement with the existing theoretical and experimental data, especially in the case of electron capture at the energy range between 10 keV and 200 keV. In addition, we presented and discussed double-differential cross sections (DDCS) as function of the ionized electron energy and its ejection angle. We showed that the majority of electrons were ionized in the forward scattering, and most of the electrons were ejected with low energies, *i.e.* less than 12 eV. The backscattered DDCSs were generally the lowest.

Finally, the 3-body classical trajectory Monte Carlo (CTMC) method was used to determine the principal quantum number (n) and the orbital angular momentum quantum number (l) dependent charge exchange (CX) cross sections for sodium atom and carbon ion collisions [4]. The projectile carbon ion charge state was taken into account from the single charge till the fully stripped ion state. We performed the calculations for 35 keV and 50 keV impact energies.
We found that higher the charge state higher value of n shows the maximum cross sections. In the similar fashion, for high n capture states the maximum l capture cross sections also shift toward to higher values of l. Moreover, we found that the CTMC modelling and the experiments on the alkali beam of stellarator Wendelstein 7-X agree that for $q = 6$ carbon ions the electron capture to the $n = 8$ state occurs with the largest probability, while in case of the $q = 5$ carbon ions the same holds for the $n = 7$ states. The CTMC calculations indicate that in these cases the cross sections have a positive correlation with l.

Publications

1. M. Al-Ajaleen, A Taoutioui and K. Tőkési. "Charge transfer and ionization cross sections in collisions of singly charged lithium ions with helium and nitrogen atoms", *Plasma Physics and Controlled Fusion* **65** (2023) 065002.

2. M. Al-Ajaleen and K. Tőkési, "Total and differential ionization cross sections in collision between nitrogen atom and singly charged sodium ion", *Scientific Reports* **13** (2023) 14080.

3. Musab Al-Ajaleen and Károly Tőkési, "Interaction of Protons with Noble-Gas Atoms: Total and Differential Cross Sections", *Atoms* **12**, 28 (2024).

4. B. G. Csillag, G. Anda, G. Cseh, D. Dunai, O. P. Ford, E. Flom, D. Gradic, F. Henke, M. Krychowiak, D. Nagy, M. Otte, D. I. Réfy, K. Tőkési, M. Vécsei, S. Zoletnik, the W7-X Team,

"Charge exchange recombination spectroscopy on the alkali beam of Wendelstein 7-X Special Collection", *Proceedings of the 25th Topical Conference on High-Temperature Plasma Diagnostics, Rev. Sci. Instrum.* **95**, 073524 (2024).

Zhongshi YANG, Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China

The radiative divertor is an effective method for controlling divertor heat flux in tokamaks. However, excessive core impurity radiation can negatively impact confinement. In recent EAST experiments, the compatibility of divertor detachment and impurity control with good core confinement have been achieved simultaneously by combining an upstream deuterium (D_2) puff and divertor argon (Ar) seeding. Experimental and SOLPS-ITER modeling results reveal that the additional D_2 puff helps mitigate target heat load and promote detachment. The enhanced divertor impurity retention from the D_2 puff is the primary reason for deeper detachment and reduced core contamination. SOLPS results also show that while the D_2 puff has a limited effect on Ar line radiation, it contributes significantly to neutral radiation in the SOL and divertor regions.

The modeling also sheds light on the physical mechanism behind the D_2 puff's impact on Ar retention. The D ions are accelerated toward the target primarily driven by the enhanced pressure gradient force and the electric field force on D. Consequently, Ar ions are accelerated toward the target driven by the frictional drag of D, which reduces backflow upstream. Increased Ar velocity is the main reason for improved Ar retention in the partial detachment state. The study also addresses challenges associated with this method. In complete detachment conditions, factors like decreased electron temperature in the divertor lead to reduced ionization of Ar and shifting of the Ar^+ ionization region upstream. These changes increase the likelihood of Ar leakage into the core, impacting Ar retention efficiency.

Publications:

Tao He, Zhongshi Yang, Kedong Li *et al.*, "Modeling Study of Divertor Pumping Effect on Detachment and Impurity Retention with Argon Seeding in EAST", *Journal of Fusion Energy* **43**:1 (2024).

Tao He, Zhongshi Yang, Kedong Li *et al.*, "Experimental and modeling study of the impact of upstream D2 puff on divertor detachment and impurity control with argon seeding in EAST", *Physics of Plasmas* **31**, 042512 (2024).

4. Future Work Plans

Haikel JELASSI, National Center of Nuclear Sciences and Technologies (CNSTN), Tunisia

During the coming two years, we will attack calculations of the electron-impact excitation concerning the low-lying levels of He-like, Lithium-like and Be-like of Ne, Ar, N and W ions. These results will be obtained using the distorted wave method (DW) implemented in FAC code. Another analytic calculation will be performed using the analytical formula of Seaton and Regemorter. A detailed comparison of the target structure will be performed to assess the uncertainty on collision strengths from the target levels. The effective collision strengths which will be obtained by averaging the electron collision strengths over a Maxwellian distribution of velocities will be addressed and tabulated for all fine-structure transitions to include up to $n = 7$ or $n = 8$ configurations, for electron temperatures T, in the range from $\log(T/\mathrm{K}) = 5$ to $\log(T/\mathrm{K}) = 7$. Detailed comparisons for the effective collision strengths will be made with the results of previous calculations such as data calculated with R-matrix method, which will pose insight on the uncertainty in their usage by astrophysical and fusion modeling.

We will also look to calculate elementary processes of He-like ions (transition metals such as Fe, Mn, Ni, Ti), since these metals occur as impurities in nuclear fusion reactors, or they are deliberately released as diagnostic tracer elements.

Atomic Parameters of all the proposed ions will be performed using both methods Multi-configuration Dirac Hartree Fock method (MCDHF) of GRASP2018 code and many-body perturbation theory (MBPT) implemented in FAC code.

Valdas JONAUSKAS, Institute of Theoretical Physics and Astronomy, Vilnius University, Lithuania

Single ionization cross sections for Ar^{+}, Ar^{3+}, Ar^{4+}, and Ar^{5+} ions are planned to be analyzed for energy levels of the ground configurations of these ions. Direct ionization (DI) and excitation-autoionization (EA) processes will be taken into account. Excitations and ionizations will be analyzed from the 3s and 3p subshells of the ground configurations. Convergence of the EA channels will be studied.

Alisher KADYROV, Faculty of Science and Engineering, Curtin University, Australia

We are currently working on and planning for 2025:

1. The total ionisation cross section and the total and n-resolved electron-capture and target-excitation cross sections in partially stripped N^{q+}, Ne^{q+} and Ar^{q+} ion collisions with ground-state atomic hydrogen and He.
2. Total and state-selective charge-exchange cross sections in fully stripped C^{6+} and N^{7+} collisions with H and He.
3. Fully differential cross sections in p, He^{2+} and C^{6+} ion collisions with H, He and H_2.

Xinwen MA, Institute of Modern Physics (IMP), Chinese Academy of Sciences (CAS), China

We are preparing to measure the charge exchange cross sections between C^{5+}, O^{5+}, N^{4+}, and N^{5+} ions and He/H_2. In addition, the charge exchange cross section measurements are also planned for Ar^{2+}, or Ar^{3+}, or Ar^{4+} ions colliding with He/H_2. Depending on the experimental resolution, one of the Ar ions will be used to conduct experiment aimed at obtaining n and l resolved state-selective cross sections. The measured cross sections will be compared with AOCC and ASCC calculations.

Sebastián OTRANTO, Instituto de Física del Sur (IFISUR), Universidad Nacional del Sur (UNS), Argentina

For the next part of the CRP, the collision processes that will be studied as defined in the 2nd Coordinated Research Meeting will be $Ar^{q+} + H(1s) \rightarrow Ar^{(q-1)+} + H^{+}$, with q = 6, 8 and $H^{+} + Ar^{q+} \rightarrow H^{(0)} + Ar^{(q+1)+}$ with q = 2 – 4. The initial impact energy range of consideration will be 1 keV/u – 100 keV/u. Since the Z-CTMC method has not been previously employed to consider the final state of the projectile, in this part of the CRP total and state-selective charge exchange cross sections will be studied with the Z-CTMC while CTMC calculations will be performed for control.

Yuri RALCHENKO, National Institute of Standards and Technology, United States of America

For the next year, primary efforts will be directed towards two projects. First, the radiative transition probabilities for the low ionization stages of Ar will be calculated using the most advanced relativistic multiconfiguration methods, e.g., the GRASP2018 package. We will also evaluate the quality and availability of atomic structure and radiative data for other impurity elements. Second, new detailed measurements of gas spectra (Ne, Ar, and possibly N) will be measured with the NIST Electron Beam Ion Trap to provide benchmark data for testing collisional-radiative models of plasma emission.

Lalita SHARMA, Indian Institute of Technology, Roorkee, India

Species	Process/Properties	Computational Procedure	Parameters of interest
Ar^{2+}	Atomic Parameters	Multi-configuration Dirac-Hartree Fock Method Many-body Perturbation Theory	Energy levels, lifetimes, wavelengths, and line strengths for electric and magnetic dipole (E1,M1) and quadrupole (E2,M2) transitions
Ar^{2+}	Electron impact excitation	Relativistic distorted wave method	Fine structure resolved cross sections, excitation rate coefficients, fitting functions for the cross sections
K-like Kr^{17+}, Xe^{35+}	Atomic Parameters	Multi-configuration Dirac Hartree Fock method and many-body perturbation theory	Energy levels, lifetimes, wavelengths, and line strengths for electric and magnetic dipole (E1,M1) and quadrupole (E2,M2) transitions
K-like Kr^{17+}, Xe^{35+}	Electron impact excitation	Relativistic distorted wave method	Fine structure resolved cross sections, excitation rate coefficients, fitting functions for the cross sections

Nicolas SISOURAT, Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France

We will complete the analysis of collisions with nitrogen ions. Furthermore, as discussed during the meeting there is a urgent need for data involving low charged argon ions. We will therefore develop potentials to treat them and we will investigate charge transfer processes between these ions and atomic hydrogen as well as proton.

Károly TŐKÉSI, HUN-REN Institute for Nuclear Research (ATOMKI)

- Total and Differential Cross Sections of Collision of Singly Charged Sodium Ions with Noble Gases
- Single and Double Ionization of Sn^{+} and Sn^{2+} by Electron Impact: Experiment and Theory
- Study on Total and *n*-resolved State-selective Cross Sections of Single Electron Capture in Ne^{8+} Collisions with H_2 and He
- Ionization Cross Sections of Hydrogen Molecule by Electron and Positron, Proton and Antiproton Impact

- Differential Ionization cross sections of Argon: Effects Due to Projectile Charge Dependent Kinematics

Our planned work will base on the 3-body classical trajectory Monte Carlo (CTMC) method. The CTMC method is a non-perturbative method, based on the calculation of a large number of individual particle trajectories when the initial atomic states are chosen randomly. In the present work, the CTMC simulations are made in the three-body approximation, where the many-electron target atom was replaced by a one-electron atom and the projectile is taken into account as one particle. The three particles are characterized by their masses and charges. The interactions among the particles are characterise with Garvey-type model potential or with Coulomb ones The initial conditions of the individual collisions are chosen at sufficiently large inter-nuclear separations from the collision centre, where the interactions among the particles are negligible. The classical equations of motion were integrated with respect to the time as independent variable by the standard Runge-Kutta method.

Zhongshi YANG, Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China

The work plan connected the CRP will include: (1) Experimental study on the interactions between injected impurities and ELMs during the radiative divertor operation on EAST. This program focuses on investigating the interactions between impurity gas injection and Edge Localized Modes (ELMs) during the H-mode discharge. By studying how impurity injection can mitigate the burst effects of ELMs on divertor target plates in terms of particle and heat flux, this research also analyzes the impact of impurity transport on the pedestal region and core plasma. (2) Continued SOLPS Simulations of Radiative Divertor Experiments. This program extends the SOLPS simulations of radiative divertor experiments, focusing on the physical mechanisms behind divertor detachment under impurity injection conditions.

5. Collaborative Activities

Two connected activities are planned which focus on low-charge states of Ar. The aim will be for an in-person Workshop at IAEA HQ to review the results of these activities in Q4 2025.

5.1 Structure and Radiative Characteristics of Low-Charge States of Argon

Participants: Y. Ralchenko (NIST, USA), V. Jonauskas (Vilnius University, Lithuania), L. Sharma (IIT Roorkee, India), C. Ballance (QUB, UK), H. Jelassi (CNTN, Tunisia). Coordinated by C. Ballance.

Introduction:

It is proposed that the first three ion stages of Argon be investigated from an atomic structure point of view using a variant of the GRASP (General Relativistic Atomic Structure Package) code. All participants have some experience or publication history with this code. The goal is to improve the theoretical values for the energy levels and the Einstein A-values for these three ion stages.

Secondary goals include improving the ionisation from the ground state and metastable levels of these three ion stages. In this regard Valdas Jounaukas will carry out distorted wave calculations and compare with the RMPS results of Connor Ballance. Then Ar II shall be investigated.

A further goal would involve Dr Martin O'Mullane (Strathclyde University, UK), who would implement these updates within ADAS (Generalized collisional radiative coefficients) that would subsequently be employed by ITER plasma modellers (ie such as within SOLPS-ITER). Having level-resolved adf04 files for the entire Argon sequence should improve the accuracy of future modelling.

Activities:

- Calculations of energy levels and Einstein *A*-coefficients of Ar II – IV; including inner shell transitions (relevant to injection of Ar into the core plasma for disruption mitigation). Insufficient data exist at present to properly model radiative processes occurring under these conditions. This activity will conduct GRASP2K calculations with relativistic effects included.

- Review of ADAS data (with M. O'Mullane) and determination of radiative power loss under relevant plasma conditions.
- Comparison of Ar II ionization with DW / FAC and R-matrix methods (C. Ballance, V. Jonauskas, K. Tőkési, H. Jelassi).

5.2 Charge Exchange involving Impurities Injected to Promote Plasma Confinement

As a collaborative activity within the CRP, we will investigate the following reactions:

(1) $H^+ + Ar^{q+} \rightarrow H^{(0)} + Ar^{(q+1)+}$

(2) $H^{(0)} + Ar^{q+} \rightarrow H^+ + Ar^{(q-1)+}$

using different theoretical approaches.

The motivations for this activity are two-fold: (1) the cross sections obtained from this work will be relevant for modelling the production of high-energy fuel neutrals which can sputter W at > 150 eV and lead to core plasma degradation; and (2) the accurate cross sections will provide a better prediction of the impurity ionization balance in fusion plasma and match experimental measurements.

The planned activities are the following:

- The development of model potentials to study collisions of low-charge Ar ions with H^+ and $H^{(0)}$.
- The computations of charge exchange cross sections for collisions between Ar^{q+} with H and H^+ using different theoretical approaches: Classical Trajectories Monte Carlo by K. Tőkési (ATOMKI, Hungary), Asymptotic-States Close-Coupling by N. Sisourat (Sorbonne U., France), Classical Trajectories Monte Carlo by S. Otranto (IFISUR, Argentina) and Wave-Packet **Convergent** Close-Coupling by A. Kadyrov (Curtin U., Australia).

Computing these cross sections represents a challenging task. The comparison between different theoretical approaches is therefore essential to provide accurate data. It should also be mentioned that there will be possible comparison with measurements at higher energy (≥1 keV/u) performed by X. Ma (IMP-CAS, China) in the coming years.

Appendix 1

List of Participants

Kalle HEINOLA, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

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Appendix 2

Agenda

Wednesday, 18 December 2024

10:00 – 10:30 **Arjan KONING** (SH-NDS), **Christian HILL**, **Kalle HEINOLA** (IAEA): Meeting Opening and Welcome; CRP background and objectives.

10:30 – 11:00 **Valdas JONAUSKAS**, *Vilnius University, Lithuania*
Electron impact ionization for neon ions

11:00 – 11:30 Coffee Break

11:30 – 12:00 **Alisher KADYROV**, *Faculty of Science and Engineering, Curtin University, Australia*
Ionisation and state-selective charge-transfer cross sections for injected impurities

12:00 – 12:30 **Xinwen MA**, *Institute of Modern Physics, Chinese Academy of Sciences (IMPCAS), China*
Benchmark measurements on $n\ell$-state-resolved cross sections in ion-atom collision processes

12:30 – 14:00 Lunch

14:00 – 14:30 **Sebastián OTRANTO**, *Instituto de Física del Sur (IFISUR), Universidad Nacional del Sur (UNS), Argentina*
State-selective charge exchange processes between Ar and Ne ions with H (1s) and H*(n = 2)

14:30 – 15:00 **Yuri RALCHENKO**, *National Institute of Standards and Technology, United States of America*
Spectroscopy of injected impurities: fundamental atomic data and collisional-radiative modeling

15:00 – 15:30 **Lalita SHARMA**, *Indian Institute of Technology, Roorkee, India*
Atomic structure properties and electron impact excitation of impurity ions

15:30 – 16:00 **Nicolas SISOURAT**, *Laboratoire de Chimie Physique – Matière et Rayonnement (LCPMR), Sorbonne Université, France*
Charge exchange cross sections in nitrogen ions and hydrogen collisions

16:00 – 16:30 Coffee Break

16:30 – 17:30 All: Discussion and planning

19:00 – 21:00 Social Dinner

Thursday, 19 December 2024

10:00 – 10:30 **Haikel JELASSI**, *National Center of Nuclear Sciences and Technologies (CNSTN), Tunisia*
Extensive Atomic Structure Calculations and Study of Plasma Parameters using Line Intensity Ratios for the Spectra Ne VIII, Fe XXIV and Kr XXXIV in The Lithium Isoelectronic Sequence

10:30 – 11:00 **Károly TŐKÉSI**, *HUN-REN Institute for Nuclear Research (ATOMKI), Hungary*
Interaction of helium and nitrogen atoms with singly charged lithium ion

11:00 – 11:30 Coffee Break

11:30 – 12:00 **Zhongshi YANG**, *Institute of Plasma Physics, Chinese Academy of Sciences (ASIPP), China*
Experimental and modeling study of the impact of upstream D_2 puff on divertor detachment with argon seeding in EAST

12:00 – 12:30 **Connor BALLANCE**, *Queen's University Belfast, United Kingdom*
R-matrix electron-impact excitation of W^{2+} and W^{6+}

12:30 – 13:00 **Christian HILL**, *IAEA, Austria*
Atomic and Molecular Data resources at the IAEA

13:00 – 14:00 Lunch

14:00 – 16:00 All: Discussion

Friday, 20 December 2024

10:00 – 13:00 Discussion: Workplan Summaries, potential Code Comparison and Benchmarking Activities;

Meeting Close

Appendix 3

Presentation Abstracts

R-matrix electron-impact excitation of W^{2+} and W^{6+}

Connor Ballance, Niall McElroy, Michael McCann, Andrew White, Catherine Ramsbottom, Stuart Loch

School of Maths and Physics, Queen s University of Belfast, Belfast, U.K., BT7 1NN
Department of Physics, Auburn University, Auburn, AL 36849, USA

A progress report of recently published electron-impact excitation and ionization work using the parallel DARC (Dirac Atomic R-matrix Codes) for W^{2+} [1] and W^{6+} [2] shall be given. Electron-impact excitation for doubly ionised Tungsten [1] has been compared with observations taken at the CTH (Compact Toroidal Hybrid) experiment at Auburn University.

Synthetic spectra as a result of Collisional Radiative (CR) modelling reveals good agreement with strong line identification of Lawson et al [3] and simple line ratios suggests lines that may offer temperature and density diagnostics. As we have data sets for both excitation and ionization of W^{2+}, S/XB ratios may be determined, whereas W^{6+} allows comparison with the spectral observations of Lawson et al. [3] from JET and other magnetically confined experiments.

References

[1] M McCann et al. 2024 *J. Phys. B: At. Mol. Opt. Phys.* **57** 235202
[2] Niall McElroy et al, *to be submitted*
[3] K Lawson et al, *Phys. Scr.* **97** (2022) 055605: https://doi.org/10.1088/1402-4896/ac5eff

Extensive Atomic Structure Calculations and Study of Plasma Parameters using Line Intensity Ratios for the Spectra Ne VIII, Fe XXIV and Kr XXXIV in The Lithium Isoelectronic Sequence

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Extensive and accurate computations have been conducted on the energy levels, wavelengths, weighted oscillator strengths, transition rates, line intensity ratios and plasma parameters for the lowest 35 odd and even parity states arising from the $1s^2\ nl$ ($n = 1 - 6$, $0 \leq l \leq n - 1$) configurations of lithium-like neon, iron, and krypton. These calculations involved the Multiconfigurational Dirac-Hartree-Fock (MCDHF) method followed by the Relativistic Configuration Interaction (RCI) approach. Transition rates were also determined for electric-multipole (dipole (E1), quadrupole (E2)) and magnetic-multipole (dipole (M1), quadrupole (M2)). The calculations incorporated Breit interactions and quantum electrodynamics effects (QED) as perturbations within the extensive relativistic configuration interaction (RCI) approach. Our results were compared with other existing theories in the literature and the data from the NIST database revealing a significant level of agreement. Additionally, the line intensity ratios and plasma parameters specifically, plasma temperature and electron density were determined. Almost all atomic data of Li-like ions presented in this paper are calculated for the first time especially those for Fe XXIV and Kr XXXIV.

Electron impact ionization for neon ions

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In this talk, the main results of the study on the single ionization process in Ne^{2+}, Ne^{3+}, and Ne^{4+} ions will be presented. Calculations are performed for the energy levels of the ground configurations of these ions. The study includes direct ionization (DI) and excitation-autoionization (EA) processes contributing to the single ionization cross sections. The distorted wave (DW) approximation, implemented in the Flexible Atomic Code (FAC) [1], is used to calculate collisional ionization and excitation cross sections. Excitations and ionizations are analyzed from the 2s and 2p subshells of the ground configurations. Convergence of the EA channels is estimated by analyzing excitations up to shells with the principal quantum numbers $n \leq 20$.

The DW approximation produces overestimated cross sections compared to measurements for the Ne^{2+} and Ne^{3+} ions. Therefore, the scaled DW cross sections [2] are used in this study to explain measurements for these ions. Additionally, the value of the single ionization threshold provided by NIST is incorporated into the study to obtain the final ionization cross sections for Ne^{2+}. The EA process contributes ~16% and ~8% to the total ionization cross sections from the ground levels of Ne^{2+} and Ne^{3+} ions, respectively. A good agreement with experimental data is obtained for the single ionization cross sections.

Our study of single ionization cross sections for the Ne^{4+} ion using the DW approximation shows a good agreement with experimental data for the four lowest energy levels of the ground configuration [3]. Excitations from the 2p subshell lead to configurations below the ionization threshold for the Ne^{4+} ion and, therefore, do not contribute to the single ionization process. The indirect ionization process contributes ~12% to the total ionization cross sections for the ground level of the ion. The DI 2p channel dominates for all studied ions.

References

[1] M. F. Gu, Can. J. Phys. 86, 675 (2008)
[2] V. Jonauskas, Astron. Astrophys. 620, A188 (2018)
[3] A. Kynienė, Š. Masys, V. Jonauskas, J. Quant. Spectrosc. Radiat. Transfer 330, 109224 (2025).

Ionisation and state-selective charge-transfer cross sections for injected impurities

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Recent progress in applications of the two-centre wave-packet convergent close-coupling (WP-CCC) approach to collisions involving injected impurity ions is reviewed. The approach uses a pseudopotential to model interactions of the multi-electron impurity ions with the target. The method has been applied to calculate the total ionisation and state-resolved electron-transfer and target-excitation cross sections in C^{2+} and C^{3+} collisions with atomic hydrogen. The total electron-capture cross sections, calculated in a broad projectile energy range from 1 keV/u to 1 MeV/u, agree with available experimental data. Charge exchange in collisions of Ar^{16+} ions with hydrogen has also been investigated. For this projectile, capture into states with $n = 14 - 17$, where n is the final-state principal quantum number, are found to be the most important. The results appear to disagree with the CTMC ones. Preliminary results for the N^{Z+} and O^{Z+} ions are also discussed.

Benchmark measurements on $n\ell$-state-resolved cross sections in ion-atom collision processes

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With the improvements of the reaction microscope installed at the 320 kV platform at the Institute of Modern Physics, a series of (n,ℓ) resolved charge exchange cross section has been measured. The models generally used in astrophysical modelling are tested in the projectile energy range from 1 to 70 keV/u, and it is demonstrated that the models are not able to describe the ℓ-population dependent on impact energy. Furthermore, our experimental result and theoretical calculations clearly demonstrate the breakdown of spin statistics assumptions at high impact energies where they are traditionally expected to be valid.

State-selective charge exchange processes between Ar and Ne ions with H (1s) and H*(n = 2)

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In this talk we will describe our advances in the proposed research program, namely the calculation of state-selective charge exchange cross sections following the collision of Ne^{10+} and Ar^{18+} ions with H(1s) and H*(n = 2) targets. The methodology employed by our group is based on the classical trajectory Monte Carlo (CTMC) method. Following up our former studies for projectile charges +6, +7 and +8, for H(1s) we have compared and analyzed the cross sections predicted by three methodologies: the standard CTMC [1], the E-CTMC [2,3] and the Z-CTMC [4,5] methods. While the CTMC method initializes the target by means of the microcanonical distribution, the E-CTMC and Z-CTMC methods employ nuclear charge and binding energy distributions to extend the radial electron distribution beyond the classical turning point. The impact energy range considered in our study was 100 eV/u – 300 keV/u. For H(1s), we have benchmarked our results with data reported with the AOCC, TC-AOCC and WP-CCC methods [6-9]. Present Z-CTMC results show good agreement with reported experimental total electron capture cross sections and are in excellent concordance at the state-selective level with available semiclassical and quantum theories. For H*(n = 2), currently under way, we compared our CTMC and Z-CTMC results to those provided by the AOCC [6,7]. Preliminary results will be presented.
As a complementary critical analysis of the classical trajectory Monte Carlo methods hereby employed, we will also show state-selective charge exchange cross sections for collisions between highly charged projectiles and H_2 [10], for which COLTRIMS experimental data have recently turned available. Our results show that from the three methods considered, the Z-CTMC is the one that better reproduces the experimental trends.

[1] R. E. Olson, A. Salop, Phys. Rev. A 16, 531 (1977).
[2] D. Eichenaur, N. Grün and W. J. Scheid, J. Phys. B 14, 3929 (1981).
[3] D. J. W. Hardie and R. E. Olson, J. Phys. B 16, 1983 (1983).
[4] N. D. Cariatore, S. Otranto and R. E. Olson, Phys. Rev. A 91, 042709 (2015).
[5] N. D. Cariatore, S. Otranto and R. E. Olson, Phys. Rev. A 93, 066702 (2016).
[6] K Igenbergs, PhD Thesis, Technische Universitt Wien (2011).
[7] D. R. Schultz, Teck-Ghee Lee and S. D. Loch, J. Phys. B 43, 144002 (2010).
[8] L. Liu, Y. Wu, J. Wang and R. Janev Atomic Data and Nuclear Data Tables 143 101464 ISSN
0092-640X, (2022).
[9] A. M. Kotian, C. T. Plowman, I. B. Abdurakhmanov, I. Bray and A. S. Kadyrov, J. Phys. B 55 115201, (2022).
[10] N. D. Cariatore and S. Otranto, Phys. Rev. A 110, 032805 (2024).

Spectroscopy of injected impurities: fundamental atomic data and collisional-radiative modeling

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Since the First Research Coordination Meeting of the CRP, a number of new and/or updated atomic parameters related to injected impurities were added to the NIST Atomic Spectra Database (ASD) [1]. ASD has been extensively updated twice (December 2023 and November 2024) bringing the total number of spectral lines to almost 301,000 transition probabilities to 129,000 and energy levels to more than 120,000. We will summarize the new additions for the first-row and noble gas atoms and ions and describe other improvements and novel features in ASD.

Also, collisional-radiative (CR) modeling for several of injected impurities will be reported with regard to spectra simulations in a typical plasma of an electron beam ion trap (EBIT). In EBITs, various gases such as nitrogen, neon and xenon are often used for spectroscopic calibration and a proper identification of their spectral lines becomes imperative. While quasi-monoenergetic electron energy distribution function in an EBIT is different from a Maxwellian distribution in tokamaks and stellarators, nonetheless, detailed spectral modeling for EBIT plasmas can reliably benchmark CR codes of a more general nature. Examples of such modeling for injected impurity gases in the NIST EBIT will be presented and discussed.

[1] URL https://www.nist.gov/pml/atomic-spectra-database

Atomic- structure properties and electron impact excitation of impurity ions

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In the research coordination meeting, I will present our progress on the computational implementation of the relativistic distorted wave theory (RDW) for calculating excitation rate coefficients within the Jena Atomic Calculator (JAC) toolbox. To address the need for large-scale calculations involving complex shells and heavy atoms and ions, we incorporated parallel programming to expedite the computation of cross sections, collision strengths, effective collision strengths and rate coefficients which are crucial for modelling various laboratory and astrophysical plasmas. Enhancements to input parameter flexibility have made the JAC more user-friendly, enabling efficient electron-impact excitation (EIE) calculations for all atoms and ions, including impurity ions relevant to our project.

Further, our detailed results will be presented on the atomic-structure properties and electron impact excitation of impurity ions. In particular, we focused on highly charged Ar-like Kr^{18+} and S-like Xe^{38+}. For Kr XIX, we focused on the lowest 128 fine-structure levels originating from the $3s^23p^6$, $3s^23p^53d$, $3s3p^63d$ and $3s^23p^43d^2$ configurations. In case of S-like Xe^{38+}, the lowest 75 levels that belong to $2s^22p^63s^23p^4$, $2s^22p^63s3p^5$, $2s^22p^63s^23p^23d^2$, $2s^22p^63s3p^43d$ and $2s^22p^6\ 3s^23p^33d$ configurations were considered. We reported energy levels, lifetimes, wavelengths, weighted oscillator strengths, and transition probabilities for multipole transition types (E1, E2, M1, and M2). To achieve this, we employed the GRASP2018 code, which implements the fully relativistic multiconfigurational Dirac–Hartree–Fock method (MCDHF) and accounts for Breit interaction and quantum electrodynamic effects. We performed another set of calculations using the many-body perturbation theory implemented in the flexible atomic code (FAC). By comparing the results obtained from GRASP2018 and FAC, we established the accuracy and consistency of our calculations. Furthermore, using the RDW theory, we studied electron impact excitation of all transitions to upper levels from the ground and metastable levels and reported EIE cross sections as a function of incident electron energies. To enhance the practical utility of our findings, we also provided analytical fittings of these cross sections and excitation rate coefficients for their applications in plasma modelling. Our work contributes to the atomic properties and excitation cross sections of Ar-like Kr^{18+} and S-like Xe^{38+}, addressing a marked gap in the available atomic data.

Additionally, we developed detailed collisional radiative (CR) models to diagnose low-temperature Kr plasma. Energies and transition parameters for Kr^{+} and Kr^{2+} were calculated using the MCDHF method. Results were compared with NIST and previously reported values to ensure accuracy. Bound state functions derived from these calculations were used to compute EIE cross sections for transitions from the five lowest levels over an electron energy range from the threshold to 300 eV, using the RDW approximation. The reliability of the CR model was confirmed through comparisons with experimental measurements.

Charge exchange cross sections in nitrogen ions and hydrogen collisions

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Within the Injected Impurities CRP, we aim to provide a consistent set of cross sections for the charge exchange processes between nitrogen ions and hydrogen atoms in a broad range of collision energies (from 1eV/u to 100 keV/u). During the talk, I will present the theoretical methods that we employ. I will then report on the results we have obtained so far, especially on the collisions of N^{4+}(2s) and N^{4+}(2p) with hydrogen.

Interaction of helium and nitrogen atoms with singly charged lithium ion

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We present a non-perturbative classical treatment of the charge transfer and ionization processes in collisions between singly charged lithium ions with helium and nitrogen atoms. Our work is a gap-filling work, as there is either very limited total cross section data are available or no available differential cross section data for this system. To model our collision systems, we used the 3-body classical trajectory Monte Carlo (CTMC) technique. The interactions among the particles are taken into account with the Garvey model potential [1]. The target was split into a single active electron and the target core consisting of the nucleus and remaining non-active electrons. The projectile was the third particle. This model potential takes into account the effective charge of the target, incorporating the screening effect of non-active electrons. In our simulations the classical equations of motion were solved numerically using the adaptive Runge-Kutta method, the step size depends on the initial parameters of all particles.

We found that, for both systems, our CTMC results for the capture process show good agreement with the previous results in the high projectile impact velocity range. Moreover, at the same time, we found that at lower impact energy range, while our total capture cross sections for helium target follows the trend of the experimental data, for the case of nitrogen target, they overestimating it a bit [2]. In addition, we also present and discuss the total ionization cross-sections of these two systems.

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References

[1] Garvey R.H. et al., Phys.Rev. A (1975) **12**, 1144.
[2] M Al-Ajaleen, et al., Plasma Phys. Control. Fusion **65** (2023) 065002.

Experimental and modeling study of the impact of upstream D_2 puff on divertor detachment with argon seeding in EAST

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This study investigates the impact of upstream deuterium (D_2) injection on impurity detachment behavior under argon (Ar) seeding conditions. Upstream D_2 injection exhibits a shielding effect on intrinsic impurities, significantly reducing core levels of tungsten (W), molybdenum (Mo), and associated radiation, demonstrating notable impurity shielding. Stable and deeper detachment was achieved under upstream D_2 injection, enabling reduced impurity accumulation in the core while maintaining good core confinement. SOLPS-ITER simulations reproduced experimental results and revealed the physical mechanisms underlying detachment enhancement and impurity shielding. D_2 injection increased impurity retention in the divertor, enhancing impurity line and neutral radiation, thus promoting detachment. Impurity retention depended on parallel impurity velocity, total ionization source intensity, ionization region shifts, and forces near the target. In partial detachment, increased impurity retention was primarily due to enhanced impurity velocity toward the target. Effective detachment and impurity shielding require optimizing the D_2 injection rate to avoid excessive impurity leakage.

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