High-Resolution X-ray Spectroscopy

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(alphabetical order)

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1 Introduction

As we have experienced with the era of diffractive grating spectrometers aboard XMM-Newton and Chandra (Brinkman et al., 2000; den Herder et al., 2001; Canizares et al., 2005), HUBS (Cui et al., 2020b,a) and other future high-resolution X-ray spectrometers will offer both an opportunity and a challenge. We will have the opportunity to greatly advance our knowledge of the Universe. We will also have the challenge to quantify key observables precisely and efficiently (Hitomi Collaboration et al., 2018; Mao et al., 2019a). To better prepare us for the upcoming new era, we need to improve the status quo in the following three aspects: atomic data, plasma models, and spectral analysis techniques. Various types of atomic data are the building blocks of plasma models. Spectral analysis techniques will take advantage of plasma models to quantify key observables.

Currently, astrophysical plasma models are mostly built on their own atomic database. APEC (Smith et al., 2001; Foster et al., 2012), ACX (Smith et al., 2012), and NEI (Smith & Hughes, 2010) are built on AtomDB[1]. CHIANTI Dere et al. (1997); Del Zanna et al. (2021) is built on its own database[2]. Cloudy (Ferland et al., 1998, 2017) used a large fraction of the CHIANTI database with some additions and modifications. SPEX (Kaastra et al., 1996, 2020) is built on SPEX-ACT (ACT is short for atomic code and tables). XSTAR (Kallman & Bautista, 2001) also has its own atomic database (Mendoza et al., 2021). Caution that the underlying atomic databases are not perfect (e.g., Mao et al., 2019b, 2022). Apart from these, there are Universal Atomic database (uaDB[3]), OPEN-ADAS[4], NIST[5] databases, etc.

[1] http://www.atomdb.org/Webguide/webguide.php
[2] https://db.chiantidatabase.org/
[3] https://heasarc.gsfc.nasa.gov/uadb/index.php
[4] https://open.adas.ac.uk/
[5] https://www.nist.gov/pml/atomic-spectra-database

Comparison among these atomic databases is not trivial. Moreover, when new theoretical calculations and lab measurements are produced by both the astro and atomic physics communities, it is not straightforward to compare new data with existing data in the aforementioned databases, let alone to estimate the impact on the interpretation of observations.

Hence, we would like to build an open atomic database for astronomers and physicists hosted at the National Astronomical Data Center (NADC)[6]. It aims to maintain atomic data from both theoretical calculations and lab measurements in a machine-readable format. The metadata, linked with publications on ADS or arXiv, is searchable and citable via a web browser. To evaluate different sources of the same type of atomic data, an integrated mapping and visualization service will be provided. The database is also expected to be accessible via a programming software package. In addition, this atomic database and its astrophysical application will also stimulate progress in the collisional theory and experimental techniques of heavy ions with neutrals in the atomic physics community in China and abroad.

Ideally, this atomic database should cover atomic data for all the elements up to Uranium (i.e., the atomic number $Z \leq 92$) since astronomers are interested in the cosmic origin of these elements (Kobayashi et al., 2020). Although the exact solar chemical composition is still not converged within the community (e.g., Anders & Grevesse, 1989; Asplund et al., 2009; Lodders et al., 2009), it is widely accepted that cosmic abundant elements include: H, He, C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, and Ni (Fig. 1). Accordingly, we aim to cover the atomic data of these elements and to provide the atomic data of other elements where possible.

Generally speaking, microscopic atomic processes among photons, electrons, ions, atoms, and molecules can be divided into collision, ionization, and recombination (Kaastra et al., 2008). Each category can be further divided into several sub-classes:

- Excitation (de-exitation)
  - Electron-impact excitation
  - Proton-impact excitation
- Recombination
  - Radiative recombination
  - Dielectron recombination
  - Multielectron recombination
- Ionization
  - Electron-impact ionization
  - Photoionization
  - Compton ionization

[6] https://nadc.china-vo.org/

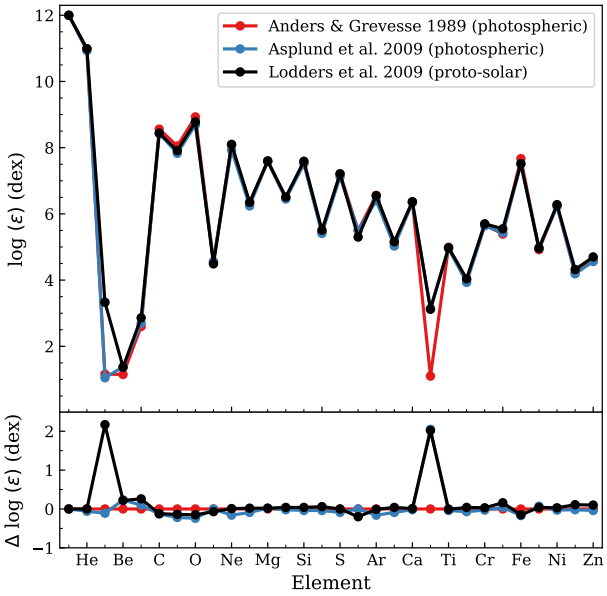

Figure 1: The present-day solar photospheric elemental abundances as a function of atomic number. The logarithmic abundance of H is defined to be log H = 12.0. Abundances of elements with $Z > 30$ are even lower than that of Zinc ($Z = 30$).

  - Autoionization and Fluorescence
  - Excitation-Autoionisation

- Charge-exchange
  - Target (H atom, other atoms, molecules)
  - Single or multiple electron capture

As a starting point, we would like to focus on (theoretical and experimental) atomic data related to atomic structure (Section 2), electron-impact excitations (Section 3), charge exchange (Section 5), and radiative recombination.

2 Atomic structure

Generally speaking, structure calculations via the Relativisitic Many-Body Perturbation Theory (RMBPT, Lindgren, 1974; Safronova et al., 1996; Vilkas et al., 1999) or Multi-Configuration Dirac-Hartree-Fock (MCDHF, Grant, 2007; Froese Fischer et al., 2016) method provide more accurate descriptions of the level energies and transition rates. Table 1 Zhang et al. (2023a) lists relevant structure calculations using RMBPT and MCDHF.

Table 1: List of atomic structure data and references Zhang et al. (2023a). Z is the atomic number and N is the number of fine-structure levels.

Begin of Table				
Sequence	Z	N	Methods	Ref.
He-like	20 – 42	49	RMBPT	Si et al. (2017)
Li-like	6	53	MCDHF	Li et al. (2021)
Be-like	6	114	MCDHF	Li et al. (2021)
	5 – 7	100	MCDHF	Wang et al. (2018a)
	8 – 10	138	MCDHF	Wang et al. (2018a)
	11 – 30	116	RMBPT	Wang et al. (2015)
	32, 36	98	RMBPT&MCDHF	Chen & Wang (2019)
	39	166	RMBPT	Chen et al. (2018)
	42	250	RMBPT&MCDHF	Chen & Wang (2018)
B-like	6	60	MCDHF	Li et al. (2021)
	16	213	RMBPT&MCDHF	Wang et al. (2018c)
	24 – 30	513	RMBPT&MCDHF	Si et al. (2018)
	36	513	RMBPT&MCDHF	Li et al. (2020)
C-like	6	100	MCDHF	Li et al. (2021)
	8	156	MCDHF	Li et al. (2022)
	9	196	MCDHF	Li et al. (2022)
	10	215	MCDHF	Li et al. (2022)
	11	272	MCDHF	Li et al. (2022)
	12	318	MCDHF	Li et al. (2022)
	13 – 36	46	MCDHF	Li et al. (2022)
	18 – 30	262	MCDHF	Ekman et al. (2014)
N-like	7	103	MCDHF	Li et al. (2023)
	18 – 30	359	RMBPT	Wang et al. (2016b)
	32	272	RMBPT&MCDHF	Wang et al. (2018a)
	34	316	RMBPT&MCDHF	Wang et al. (2018b)
	36	272	RMBPT&MCDHF	Wang et al. (2017c)
	40	272	RMBPT&MCDHF	Wang et al. (2019a)
O-like	18	156	MCDHF	Song et al. (2021)
	19	179	MCDHF	Song et al. (2021)
	20	196	MCDHF	Song et al. (2021)
	21 – 23	200	MCDHF	Song et al. (2021)
	24 – 30	200	RMBPT&MCDHF	Wang et al. (2017a)
	34	318	RMBPT&MCDHF	Chen et al. (2018)

Continuation of Table 1				
Sequence	Z	N	Methods	Ref.
	36	344	RMBPT&MCDHF	Wang et al. (2017b)
	42	318	RMBPT&MCDHF	Wang et al. (2019b)
F-like	24 – 30	200	RMBPT&MCDHF	Si et al. (2016)
	31 – 35	200	RMBPT&MCDHF	Li et al. (2019)
	36	200	RMBPT&MCDHF	Zhang et al. (2018)
Ne-like	24 – 36	201	RMBPT	Wang et al. (2016a)
Na-like	14	45	MCDHF	Atalay et al. (2019)
Na-like	18, 36, 54	71	RMBPT&MCDHF	Rathi & Sharma (2022)
Mg-like	14	106	MCDHF	Atalay et al. (2019)
Al-like	36	880	RMBPT	Zhang et al. (2018)
Si-like	24	604	MCDHF	Zhang et al. (2021)
Si-like	25	699	MCDHF	Zhang et al. (2021)
Si-like	26	702	MCDHF	Zhang et al. (2021)
Si-like	27 – 29	704	MCDHF	Zhang et al. (2021)
Si-like	30	699	MCDHF	Zhang et al. (2021)
Ca-like	26	134	MCDHF	Li et al. (2018)
End of Table				

3 Electron-impact excitation

Electron-impact excitation and de-excitation is a fundamental atomic process. As a density sensitive process, it plays an important role in both emission and absorption lines in astrophysical plasmas (e.g., Mao et al., 2017b; Hitomi Collaboration et al., 2018; Del Zanna & Mason, 2018; Mao et al., 2022; Tomaru et al., 2023).

Large-scale electron-impact excitation data are mostly calculated via the R-matrix Intermediate Coupling Frame Transformation (ICFT, Griffin et al., 1998) approach (Badnell et al., 2016). For lowly ionized ions, data calculated via the Dirac R-matrix code (DARC[7]) and B-spline R-matrix (BSR, Zatsarinny, 2006) are more accurate (e.g., Porquet et al., 2010; Mao et al., 2020a; Morisset et al., 2020; Mao et al., 2020b, 2021). Spectral lines of these ions are usually outside the X-ray band (e.g., Morisset et al., 2020). For highly ionized ions, collision data calculated via the Independent Process and Isolated Resonances approximation using Distorted Waves (IPIRDW) are consistent with those R-matrix data (e.g., Gu, 2004; Chen et al., 2010).

[7] http://amdpp.phys.strath.ac.uk/rmatrix/ser/darc/

Table 2: List of level-resolved electron-impact excitation data and references.Z is the atomic number and N is the number of fine-structure levels.

Sequence	Z	N	Method	Reference
H-like	$6-30$	36	ICFT	Mao et al. (2022)
	$13-42$	36	IPIRDW	Li et al. (2015)
He-like	$6-30$	71	ICFT	Mao et al. (2022)
	$20-42$	49	IPIRDW	Si et al. (2017)
Li-like	$4-30$	195	ICFT	Liang & Badnell (2011)
Be-like	$5-30$	238	ICFT	Fernández-Menchero et al. (2014a)
	7	238	BSR	Fernández-Menchero et al. (2017)
	7	238	DARC	Aggarwal et al. (2016)
B-like	$6-36$	204	ICFT	Liang et al. (2012)
C-like	$7-36$	590	ICFT	Mao et al. (2020a)
	8	202	BSR	Tayal & Zatsarinny (2017)
	26	590	ICFT	Fernández-Menchero et al. (2016)
N-like	$8-30$	725	ICFT	Mao et al. (2020b)
	8	21	BSR	Kisielius et al. (2009)
	8	47	BSR	Tayal (2007)
O-like	$9-30$	630	ICFT	Mao et al. (2021)
	10	554	ICFT	McLaughlin et al. (2011)
F-like	$10-36$	195	ICFT	Witthoeft et al. (2007)
Ne-like	$11-36$	209	ICFT	Liang & Badnell (2010)
Na-like	$12-36$	32	ICFT	Liang et al. (2009)
Mg-like	$13-30$	283	ICFT	Fernández-Menchero et al. (2014b)

4 Dielectronic recombination

Dielectronic recombination (DR) is the dominant electron-ion recombination process in both photoionized plasmas (PP) and collisionally ionized plasmas (CP) Zanna & Mason (2018); Dere et al. (2019); Beilmann et al. (2011); Schnell et al. (2003); Dere et al. (2019); Badnell (2006c). DR establishes the ionization balance of elemental charge-states in non-LTE plasmas. This is a basic building block for spectroscopic diagnostic modeling. Furthermore, DR satellite lines themselves can be used as temperature and density diagnostics for such plasmas Zanna & Mason (2018).

Table 3: List of dielectronic recombination data and references. Z is the atomic number.

Sequence	Z	Method	Reference
H-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	2-30,36,42,54	AS	Badnell (2006a)
He-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	3-30,36,42,54	AS	Bautista & Badnell (2007)
Li-like	12,14,16,18,20,26,28	FAC	Gu (2003); Khan et al. (2022)
	4-30,36,42,54	AS	Colgan et al. (2004)
Be-like	18	FAC&AS	Zhang et al. (2023b); Huang et al. (2018)
	12,14,16,18,20,26,28	FAC	Gu (2003)
	5-30,36,42,54	AS	Colgan et al. (2003); Wang et al. (2018b)
B-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	6-30,36,42,54	AS	Altun et al. (2004)
C-like	20	FAC&AS	Wen et al. (2020)
	12,14,16,18,20,26,28	FAC	Gu (2003); Ma et al. (2023)
	7-30,36,42,54	AS	Zatsarinny et al. (2004b)
N-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	8-30,36,42,54	AS	Mitnik & Badnell (2004)
O-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	9-30,36,42,54	AS	Zatsarinny et al. (2003)
F-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	10-30,36,42,54	AS	Zatsarinny et al. (2006)
Ne-like	12,14,16,18,20,26,28	FAC	Gu (2003)
	11-30,36,42,48,54	AS	Zatsarinny et al. (2004a)
Na-like	36	FAC&AS	Huang et al. (2020)
	12-30,36,42,54	AS	Altun et al. (2006)
Mg-like	13-30,36,42,54	AS	Altun et al. (2007)
Al-like	14-30	AS	Badnell (2006c); Abdel-Naby et al. (2012)
Si-like	15-30	AS	Badnell (2006b); Kaur et al. (2018)
P-like	16-30,36,42,54,74	AS	Badnell (2006b); Bleda et al. (2022)
S-like	26	AS	Badnell (2006b)
Cl-like	26	AS	Badnell (2006b)
Ar-like	23-30,36,42,50,54,60,64,70,74,79,85,92	FAC	Li et al. (2019)
	26	AS	Badnell (2006b)
Ni-like	79	FAC	Shi et al. (2004)
Co-like	36,42,47,54,59,66,74,79,85,92	FAC	Meng et al. (2007, 2008, 2009)
Xe-like	74	AS	Badnell et al. (2012)
Cs-like	74	AS	Badnell et al. (2016)
Rb-like to Pd-like	74	AS	Preval et al. (2018b)
Pm-like to Ta-like	74	AS	Preval et al. (2018a)

5 Charge exchange

Charge-exchange cross sections are fundamental parameter to estimate its contribution in many objects with hot plasma impacting on cold media, such as solar wind charge-exchange (e.g., Branduardi-Raymont et al., 2007), supernova remnants (e.g., Gu et al.,

2016), star-formation galaxies (e.g., Zhang et al., 2014), and clusters of galaxies (e.g., Gu et al., 2015).

Charge-exchange (CX) cross sections are best calculated by atomic-orbital close-coupling (Fritsch & Lin, 1984) and quantum mechanical molecular-orbital close-coupling methods (Nolte et al., 2012). Whereas many available data are calculated by using multichannel Landau-Zener (Janev et al., 1983), and/or classical trajectory Monte Carlo methods due to computational efficiency. In the Kronos database, the CX cross-sections of bared and H-like ions with different targets have been provided (Mullen et al., 2017; Cumbee et al., 2018), including H, He, H_2O, CO, CO_2, OH, and O, by using multichannel Landau-Zener method except for collisions with H and He atoms, where the AOCC and/or QMOCC were used.

Table 4: List of experimental charge-exchange cross section and references.

Ions	Targets	Type	Reference
C^{q+} (q=3,5,6)	CO	total[a]	Mawhorter et al. (2007)
C^{5+}	H_2O	total[a]	Mawhorter et al. (2007)
C^{q+} (3≤q≤6)	CH_4	total[a]	Djurić et al. (2008)
C^{q+} (q=3,6)	H_2, He, H_2O, CO_2	total[a]	Greenwood et al. (2001)
N^{3+}	He	LS	Xu et al. (2020)
N^{q+} (4≤q≤7)	CH_4	total[a]	Djurić et al. (2008)
N^{q+} (q=4,7)	H_2, He, H_2O, CO_2	total[a]	Greenwood et al. (2001)
N^{7+}	He, CO, CO_2, H_2O	n	Hasan et al. (2001)
N^{7+}	H	total	Zhang et al. (2022)
N^{6+}	He	n	Zhu's exp
O^{7+}	He, CO, CO_2, H_2O	n	Hasan et al. (2001)
O^{q+} (5≤q≤8)	CO	total[a]	Mawhorter et al. (2007)
O^{q+} (5≤q≤7)	CO_2	total[a]	Mawhorter et al. (2007)
O^{q+} (5≤q≤7)	CH_4	total[a]	Djurić et al. (2008)
O^{q+} (q=5,7,8)	H_2, He, H_2O, CO_2	total[a]	Greenwood et al. (2001)
O^{6+}	H_2O	total[a]	Mawhorter et al. (2007)
O^{6+}	H_2/He	n	Zhu's exp
Ne^{q+} (q=7,8)	H_2O, CO, CO_2	total[a]	Mawhorter et al. (2007)
Ne^{9+}	H, He, CO_2, H_2O	total[a]	Greenwood et al. (2001)
$Ne^{8+,9+}$	H_2 & He	n	Xu et al. (2021)
Ne^{10+}	He	n	Cassimi et al. (1996)
Ar^{18+}	He	n	Cassimi et al. (1996)

[a] Include multiple charge exchange cross section.

6 Radiative recombination

Radiative recombination can give rise to recombination lines (Osterbrock & Ferland, 2006) as well as radiative recombination continuum (RRC). The latter can be found in recombining plasmas of supernova remnants (e.g., Kawasaki et al., 2002; Yamaguchi et al., 2009; Ohnishi et al., 2011; Sawada & Koyama, 2012; Uchida et al., 2012; Sun & Chen, 2020), photoionized plasmas of X-ray binaries (e.g., Liedahl & Paerels, 1996) and Active Galactic Nuclei (e.g., Kinkhabwala et al., 2002; Mao et al., 2018).

Radiative recombination data of H- to Na-like ions with atomic number $Z \leq 30$ are mainly sourced from Badnell (2006) for the rate coefficients and Mao et al. (2017a) for the cooling rates. Both level-resolved and total rates are provided in these calculations. In addition, Mao & Kaastra (2016) provided parameterization of the rate coefficients.

7 Plasma models

The development of plasma codes and models (e.g., APEC, SPEX) mentioned in Section 1 can be traced back to the 1970s. Continuous developments of plasma codes are essential to meet the scientific goals set by ever-improving high-resolution X-ray spectrometers.

Here we would like to upgrade the existing plasma code SASAL (Liang et al., 2014b,a), which was based on the IDL programming language. SASAL can be used for plasma diagnostics of collisional ionized equilibrium (CIE), non-equilibrium ionization (NEI), and charge exchange (CX). A python version (SasalPy) with an updated atomic database is being developed to make it more friendly to the community (Hao et al. in prep.). Fig. 2 shows the flow chart of SasalPy to calculate the spectrum of CIE plasmas and a demo for the spectrum of Fe XIV at the temperature of 7.5×10^6 K. The flow chart shows the modularization feature of this plasma model that is the goal of our pursue. These modules labelled with 1-4 can be run in two different modes, e.g. rerun with updated atomic database or different temperature grids, and reading stored data files of the line emissivities and charge state distributions. The reading mode benefits the fast requirement in the global-fitting in the imaging-spectroscopy era, while the rerun mode will benefit the requirement of detail analysis with updating atomic data or with fine temperature grids. The modules of 5–8 is related to the applications for different users. Additionally, a demo of Fe XIV spectrum is presented to illustrate its easy access by different user interfaces.

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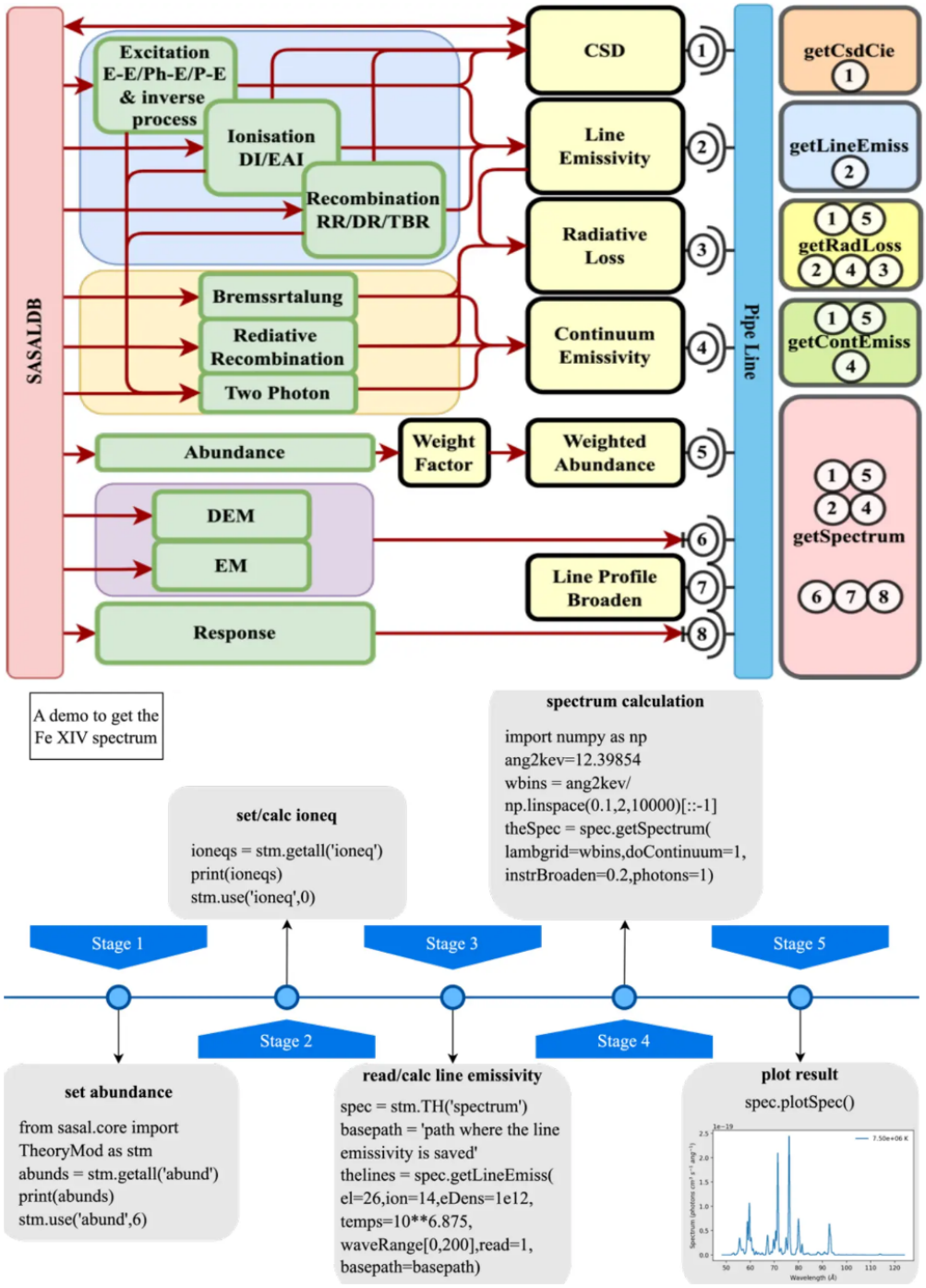

Figure 2: The flow chart (top) of the sasalPy for the collisional ionization equilibrium, and a demo (bottom) for the CIE spectrum of Fe XIV at the temperature of 7.5×10^6 K.

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