Massive Calculations of Atomic Properties with High Accuracy for Boron-like Iron and other Ions of Astrophysical Interest

J. Ekman[1], P. Jönsson[1], S. Gustafsson[1], H. Hartman[1], R. du Rietz[1], G. Gaigalas[2], M. Godefroid[3], C. Froese Fischer[4]

[1] *Group for Materials Science and Applied Mathematics, School of Technology, Malmö University, Sweden*

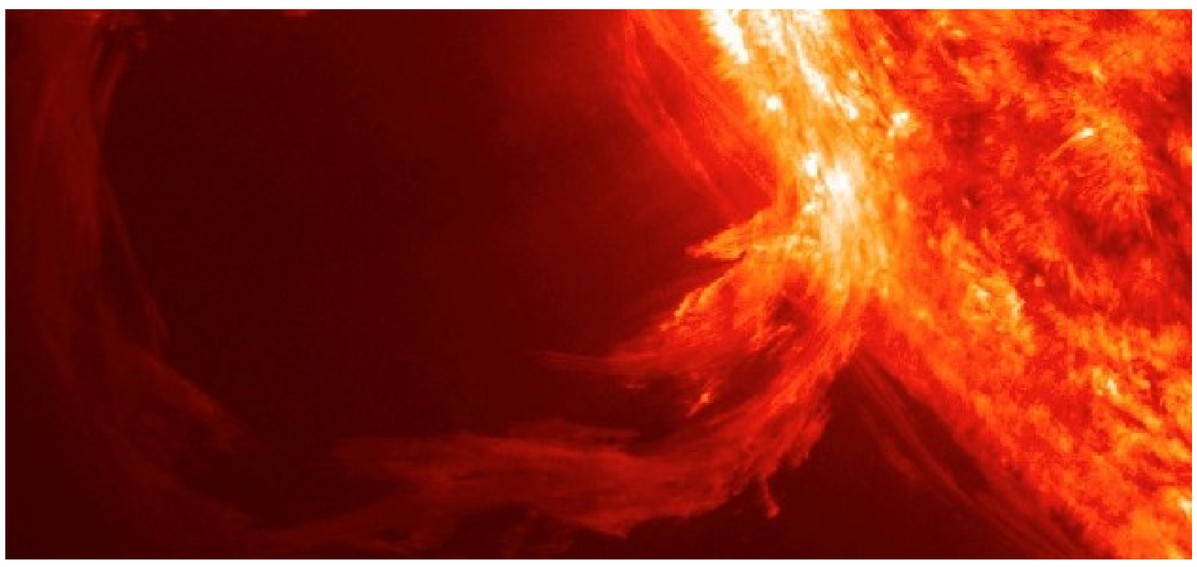
[2] *Vilnius University, Institute of Theoretical Physics and Astronomy, Lithuania*

[3] *Chimie Quantique et Photophysique, Université Libre de Bruxelles, Belgium*

[4] *National Institute of Standards and Technology, Gaithersburg, USA*

Needs for atomic data in astrophysics

Information about physical processes in astrophysical and fusion plasmas can be inferred from high resolution spectra. The X-ray spectra from iron L-shell ions are particularly important for astrophysics as they are in the wave length range covered by telescopes on board the space observatories Chandra and XMM-Newton. The analysis of high-resolution X-ray spectra requires knowledge of a large number of accurate transition data and transition probabilities, either from theory or experiment, to identify spectral lines, produce synthetic spectra, and carry out plasma diagnostics.



Spectra from highly charged ions can be observed during flares

Computer codes for atomic properties

To meet the demands for atomic data the COMPutational Atomic Structure (COMPAS) group has been formed. The group is involved in developing state of the art computer codes for atomic calculations in the non-relativistic scheme with relativistic corrections in the Breit-Pauli approximation ATSP2K [1] as well as in the fully relativistic scheme GRASP2K [2]. The codes rely on multiconfiguration methods and the wave function for an atomic state is expanded in configuration state functions (CSFs).

The advantages:

- Flexible, can be applied also to systems including open f-shells [3]
- Large part of a spectrum can be computed in one calculation
- Parallel versions of the codes allow for large expansions
- Computes a variety of bound state properties
- Output can be merged into databases

Accurate atomic calculations

The success of large scale multiconfiguration calculations for atomic systems rely on judiciously chosen configuration expansions. The configuration expansions are normally generated by the active set method. Here CSFs of a specified parity and J symmetry are generated by excitations from a number of reference configurations to a set of orbitals according to some rules (correlation model). To be able to monitor the convergence of the calculated energies and transition parameters, the active sets is increased in a systematic way by adding layers of correlation orbitals. To estimate the uncertainties in the computed properties the results are monitored with respect to the correlation model. On a desktop computer system expansions with 1 000 000 to 1 500 000 CSFs are handled without problems.

Active set method:

- Define a multireference
- Define a rule (correlation model) for excitations to the orbital set
- Increase the orbital set and monitor the convergence
- Relax the rule (include more correlation) and monitor the difference

Boron-like ions, Si X

Calculations were performed for the 291 lowest states in boron-like ions, including Si X and Fe XXII, belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$, $1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, $1s^22p^24l'$ ($l = 0, 1, 2$ and $l' = 0, 1, 2, 3$). "Spectroscopic accuracy" is attained with transition energies correct to a fraction of a per mille [4].

Label		E_{calc} (cm^{-1})	E_{obs} (cm^{-1})	Diff
$2s^22p$	$^2P_{1/2}$	0	0	0
$2s^22p$	$^2P_{3/2}$	6 990	6 991	-1
$2s2p^2$	$^4P_{1/2}$	161 022	161 010	12
$2s2p^2$	$^4P_{3/2}$	163 453	163 490	-37
$2s2p^2$	$^4P_{5/2}$	167 044	167 060	-16
$2s2p^2$	$^2D_{3/2}$	288 100	287 850	250
$2s2p^2$	$^2D_{5/2}$	288 117	287 880	237
$2s2p^2$	$^2S_{1/2}$	368 007	367 670	337
$2p^3$	$^2P_{1/2}$	646 972	646 760	212
$2p^3$	$^2P_{3/2}$	647 589	647 390	199
$2s^23s$	$^2S_{1/2}$	1 821 975	1 822 000	-25
$2s^23p$	$^2P_{1/2}$	1 902 444	1 902 100	344
$2s^23p$	$^2P_{3/2}$	1 904 304	1 903 957	347
$2s^23d$	$^2D_{3/2}$	1 979 272	1 979 260	12
$2s^23d$	$^2D_{5/2}$	1 979 762	1 979 730	32
$2p^23p$	$^2D_{5/2}$	2 435 354	2 435 260	94
$2p^23d$	$^4P_{5/2}$	2 444 419	2 444 460	-41
$2p^23d$	$^4P_{3/2}$	2 446 095	2 446 000	95
$2p^23d$	$^4P_{1/2}$	2 446 963	2 446 877	90

Carbon-like ions, Fe XXI

Calculations were performed for the 273 lowest states in carbon-like ions, including Fe XXI, belonging to the configurations $1s^22s^22p^2$, $1s^22s2p^3$, $1s^22p^4$, $1s^22s^22p3l$, $1s^22s2p^23l$, $1s^22p^33l$, $1s^22s^22p4l$, ($l = 0, 1, 2$). Also in this case "spectroscopic accuracy" is attained with transition energies correct to a fraction of a per mille [5].

Label		E_{calc} (cm^{-1})	E_{obs} (cm^{-1})	Diff
$2s^22p^2$	$^3P_0$	0	0	0
$2s^22p^2$	$^3P_1$	73 863	73 851	12
$2s^22p^2$	$^3P_2$	117 416	117 354	62
$2s^22p^2$	$^1D_2$	244 750	244 561	189
$2s^22p^2$	$^1S_0$	372 137	371 980	157
$2s2p^3$	$^5S_2$	486 583	486 950	-367
$2s2p^3$	$^3D_1$	776 775	776 690	85
$2s2p^3$	$^3D_2$	777 403	777 340	63
$2s2p^3$	$^3D_3$	803 617	803 540	77
$2s2p^3$	$^3P_0$	916 444	916 330	114
$2s2p^3$	$^3P_1$	925 073	924 920	153
$2s2p^3$	$^3P_2$	942 621	942 430	191
$2p^4$	$^3P_1$	1 740 622	1 740 500	122
$2p^4$	$^1D_2$	1 817 786	1 817 100	686
$2p^4$	$^1S_0$	2 048 511	2 048 200	311

References

[1] C. Froese Fisher et al. Comput. Phys. Commun. **176** 559 (2007).

[2] P. Jönsson et al. Comput. Phys. Commun. **184** 2197 (2013).

[3] G. Gaigalas et al. Comput. Phys. Commun. **139** 263 (2001).

[4] P. Jönsson, J. Ekman et al. A&A, accepted (2013).

[5] P. Jönsson, J. Ekman et al. A&A, in preparation (2013).