



# BalticGrid-II Project

## Investigation of Highly Charged Ions for ITER project

*Ab initio* study of ion spectral characteristics using GRID technology

Spectroscopic research is one of the most effective ways of exploring the structure, characteristics and properties of atoms and ions, and materials they form. Modern methods and technologies allow registering of high precision experimental spectra and other spectroscopic data covering all electromagnetic wave bands. However, accurate and reliable theoretical calculations are necessary to interpret the obtained data and understand the processes that happened in the radiating object.

Scientists of Department of Theory of Atom at Institute of Theoretical Physics and Astronomy of Vilnius University (ITPA VU) have been accumulating experience in developing and applying methods of theoretical spectroscopic research for a half of a century. World-wide known computer codes along with original ones created at ITPA VU are used for *ab initio* calculations of energy spectra and various transition characteristics of atoms and highly-charged ions.

High qualification of ITPA VU scientists have been acknowledged by signing the contract of Association with EURATOM within the framework of the European Fusion Development Agreement. Through the contract ITPA VU participates in one of the biggest nowadays projects ITER -

- a joint international research and development project that aims to demonstrate the scientific and technical feasibility of fusion power. ITER is planned to show that fusion could be used to generate electrical power, and to gain the necessary data to design and operate the first electricity-producing plant.

Investigation of tungsten properties is of major interest for construction of modern fusion devices, such as ITER. Tungsten is planned to be used as a plasma facing material. Due to the high specific radiation losses if the element penetrates into the central plasma region, its fractional abundance in the plasma of a fusion device should be carefully controlled. Relevant spectroscopic data are necessary to investigate behavior of tungsten and its ions in the plasma. ITPA VU scientists are performing theoretical treatment of wavelengths, transition probabilities, oscillator strengths and radiative lifetimes of tungsten for this project. High quality theoretical investigations of heavy ions with open shells are time demanding and require large computing resources. In some cases the accuracy of the calculated data is limited by the capacity of available machines. GRID technologies and infrastructure have opened new possibilities for a wide-scale theoretical research of spectral characteristics of atoms and ions.

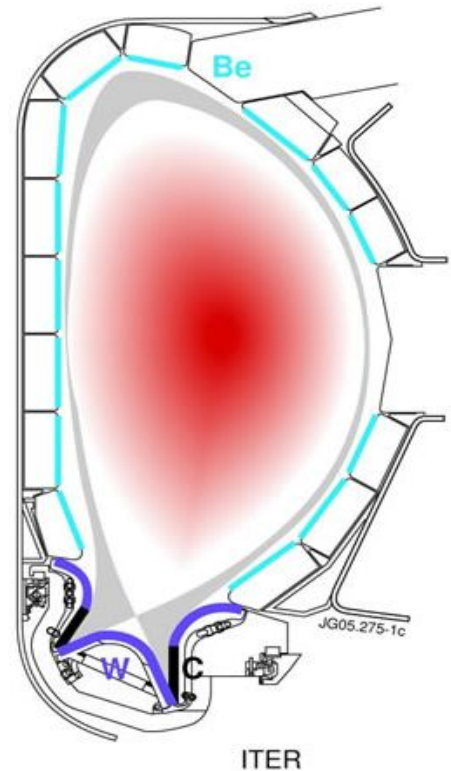


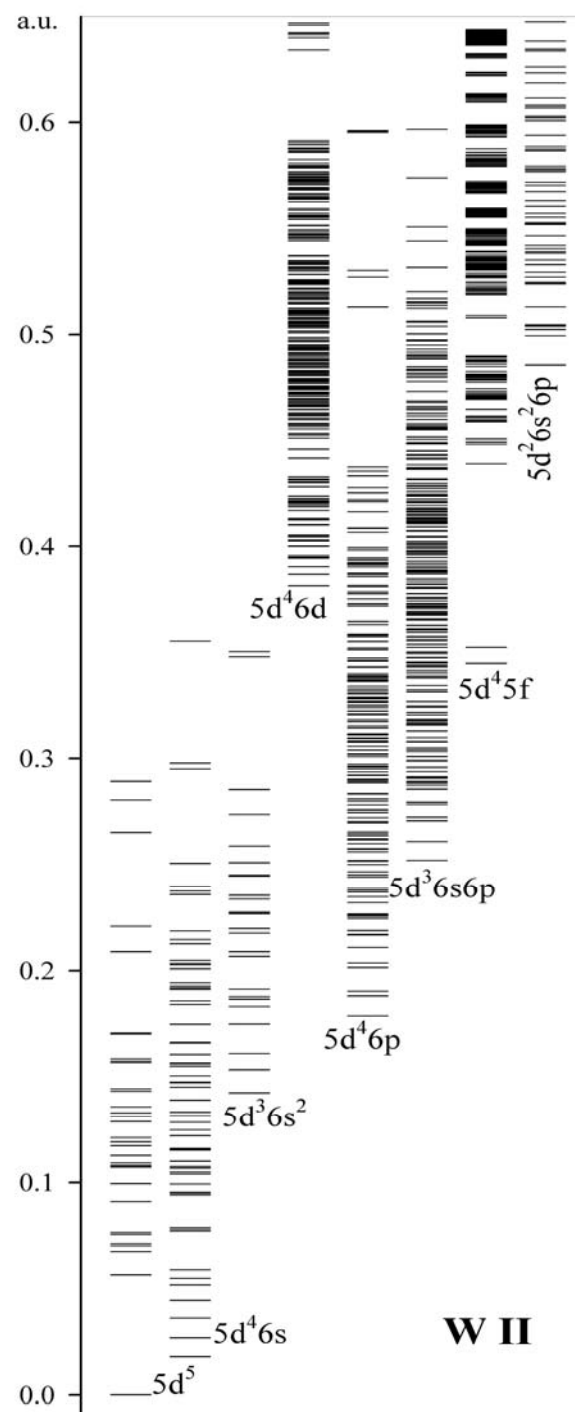
Fig. 1: Wall Project. ITER wall with tungsten used in the divertor ([www.jet.efda.org](http://www.jet.efda.org))





Theoretical *ab initio* studies of spectral characteristics of highly charged ions can be performed within two Breit-Pauli approaches using the configuration interaction method on the basis of transformed radial orbitals with a variable parameter for wide account of the correlation effects. The radial orbitals can be obtained using the code HF96 by Ch. Froese-Fischer in the non-relativistic case or our original code QRHF where the quasirelativistic approach is implemented and radial orbitals obtained are to some degree relativistic. The transformed radial orbitals describing the virtually excited electrons for configuration interaction are calculated by our original computer code TRANRO. Further the configurations are selected and the function basis is formed using our programs SELECTCONF and ATOTERM. The adapted computer program BREIT calculates the angular parts of the energy operator matrix elements. Our original code MATRFO is used to form and diagonalize the energy matrices. Finally, the computer codes MLTIPO and LSJTRN are used to calculate the matrix elements of the transition operator and derive the transition characteristics.

Due to specific properties of thermonuclear plasma, tungsten ions of various ionization degrees appear in the fusion device. The ground and first excited configurations of the tungsten ions important for thermonuclear plasma modeling (for example, W II ion) contain many open shells including 4f and 5d ones. In such a case a large number of angular coefficients need to be calculated. Also one configuration with an open shell can contain hundreds of levels. Seeking to obtain high accuracy results it is necessary to take into account a thousand of admixed configurations. Thus the number of angular coefficients within the calculation exceeds one million and the energy operator matrices appear to be of the order of some tens of thousands. Such theoretical investigation would be nearly impossible without the computational resources that are available through BalticGrid-II and LitGrid infrastructures.



**Fig. 2:** Energy spectra of the ground and first excited configurations of tungsten ion W II

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