

PAPER • OPEN ACCESS

## Combined MCDHF-CI and MBPT calculations for $n=4$ to $n=3$ x-ray transitions in Ni-like tungsten

To cite this article: K Koziol and J Rzadkiewicz 2020 *J. Phys.: Conf. Ser.* **1412** 132021

View the [article online](#) for updates and enhancements.

### You may also like

- [Energy levels, transition rates, oscillator strengths and lifetimes in Ne-like, Ni-like, and Cu-like uranium ions](#)  
M A Bari, R T Nazir, M H Nasim et al.
- [Spectroscopy of M-shell x-ray transitions in Zn-like through Co-like W](#)  
J Clementson, P Beiersdorfer, G V Brown et al.
- [Identifications of extreme ultraviolet spectra of Br-like to Ni-like neodymium ions using an electron beam ion trap](#)  
C Suzuki, Dipti, Y Yang et al.



**ECS**  
The  
Electrochemical  
Society  
Advancing solid state &  
electrochemical science & technology

**DISCOVER**  
how sustainability  
intersects with  
electrochemistry & solid  
state science research

## Combined MCDHF-CI and MBPT calculations for $n=4$ to $n=3$ x-ray transitions in Ni-like tungsten

K Koziol\* and J Rządiewicz†

National Centre for Nuclear Research (NCBJ), Andrzej Soltana 7, 05-400 Otwock-Świerk, Poland

**Synopsis** The  $4d \rightarrow 3p$ ,  $4p \rightarrow 3s$ , and  $4f \rightarrow 3p$  x-ray transitions in Ni-like tungsten ions have been studied theoretically. The Multiconfiguration Dirac–Hartree–Fock method and the large-scale relativistic Configuration Interaction and Many Body Perturbation Theory methods have been employed in order to take into account electron correlation effects on the lines wavelengths.

Tungsten is chosen as a plasma facing material in modern large tokamaks, such as JET and ITER. Therefore, spectroscopic studies of tungsten ions are a tool for diagnostics relevant for a wide range of electron temperatures [1].

**Table 1.** Wavelengths of Ni1, Ni2, and Ni3 transitions (Å) for various theoretical approaches.

	Ni1	Ni2	Ni3
AMBIT:			
MCDHF	5.1986	5.2528	4.6394
+CI	5.2007	5.2537	4.6420
+CI+MBPT	5.2011	5.2543	4.6424
GRASP2K (cited from Ref. [2]):			
MCDHF	5.1947	5.2486	4.6367
+CI(FCI)	5.1994	5.2517	4.6519
+CI(FCI*)	5.1988	5.2510	4.6413
+CI(CV)	5.2010	5.2541	4.6318
+CI(CV*)	5.2004	5.2532	4.6417
Experiment:			
Ref. [3]	5.2008(3)	5.2540(3)	
Ref. [4]	5.2002(9)	5.2520(16)	4.6372(10)

In our previous paper [3] the x-ray transitions in Ni- and Cu-like tungsten ions in the 5.19–5.26 Å wavelength range that are relevant as a high-temperature tokamak diagnostic have been studied. In our next paper [2] various Multiconfiguration Dirac–Hartree–Fock (MCDHF) plus Configuration Interaction (CI) approaches (named FCI, FCI\*, CV, and CV\* in Table 1; see [2] for detailed description), employing GRASP2K [5] code, have been tested in order to reproduce and predict experimental wavelengths of  $4d \rightarrow 3p$  transitions in Ni- and Cu-like tungsten ions.

\*E-mail: Karol.Koziol@ncbj.gov.pl

†E-mail: Jacek.Rzadkiewicz@ncbj.gov.pl

In the present work the calculations of the wavelengths of the  $4d \rightarrow 3p$ ,  $4p \rightarrow 3s$ , and  $4f \rightarrow 3p$  x-ray transitions in Ni-like tungsten ions have been carried out by means of the AMBIT [6] code, based on MCDHF method with CI and Many Body Perturbation Theory (MBPT) approaches in order to take into account electron correlation effects on the lines wavelengths. Applying both the MCDHF-CI and the MCDHF-CI + MBPT approaches instead the “pure” MCDHF approach allowed to reduce substantially the experiment–theory gap in wavelengths. Results of this study provide an important benchmark for x-ray measurements in tokamaks.

**Acknowledgments:** The work was partly supported by the Polish Ministry of Science and Higher Education within the framework of the scientific financial resources in the years 2016–2019 allocated for the realization of the international co-financed project. This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom Research and Training Programme 2014–2019 under Grant Agreement No. 633053.

### References

- [1] Pütterich T, Neu R, Dux R *et al* 2008 *Plasma Phys. Controlled Fusion* **50** 085016
- [2] Koziol K and Rządiewicz J 2018 *Phys. Rev. A* **98** 062504
- [3] Rządiewicz J, Yang Y, Koziol K *et al* 2018 *Phys. Rev. A* **97** 052501
- [4] Clementson J, Beiersdorfer P, Brown G V, and Gu M F 2010 *Phys. Scr.* **81** 015301
- [5] Jönsson P, Gaigalas G, Bieroń J, Froese Fischer C, and Grant I P 2013 *Comput. Phys. Commun.* **184** 2197
- [6] Kahl E V and Berengut J C 2018 *Comput. Phys. Commun.* **238** 232

