§16. *Ab initio* Multi-configuration Dirac-Fock Calculation of M1 Visible Transitions among the Ground State Multiplets of the W^{26+} Ion

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Tungsten (W) is currently considered to be a good candidate for the surface material of the divertor and main chamber plasma facing components in future magnetic fusion devices due to its refractory properties. However, using tungsten as a shield material, tungsten atoms and ions will inevitably be introduced into the plasma as an intrinsic impurity. Due to their large radiation loss, tungsten impurity ions will be deleterious for the achievement of the ignition in magnetically confined fusion. To diagnose, understand and control the influx of impurity tungsten ions, a thorough knowledge of atomic physics on tungsten ions will be helpful.

Recently, we observed visible spectra of moderately charged tungsten ions using a compact EBIT (coBIT) at electron energies of 200-1000 eV and found many previously unreported lines. Among these lines, a strong line at 389.41 nm, observed with the electron beam energy of 870 eV, was attributed to the emission from W^{26+}. Theoretically the ground state configuration of W^{26+} is $[Kr]4d^{10}4f^2$, which is one of the simplest examples of a complex configuration with multiple 4f electrons. For such a heavy element with nuclear charge Z=74, a relativistic treatment is desired. Meanwhile, the moderately ionized ions still have a substantial number of electrons, which repel each other via the Coulomb force and lead to a complex electron correlation.

The present calculation was performed in the framework of the multi-configuration Dirac-Fock (MCDF) method with the implementation of GRASP2K[1] and RATIP packages. In order to take the most important electron correlation effects into account, a systematical single and double substitution from 4d and 4f orbital to a restricted active space (AS) was employed. The Breit interaction, vacuum polarization and self-energy effects are estimated by the relativistic configuration interaction calculation considering the Dirac-Fock-Breit Hamiltonian matrix in terms of configuration state functions with a fixed orbital basis set. The Breit interaction was usually considered in the low-frequency limit.

To investigate the correlation contributions, two strategies of calculation for the structure of the ground state of W^{26+} are implemented. The method A considers only the VV (valence-valence) and CV (core-valence) correlations while the method B considers also CC (core-core) correlation contributions.

According to our theoretical estimation, there is only one transition near the observed wavelength, which is the M1 transition of $^3H_5 \rightarrow {}^3H_4$ of the W^{26+} ion ground states. The calculated wavelength of this transition in different methods and AS is presented in Fig 1. The calculated wavelength by method B is quickly converged to 388.43 nm which is only 0.3% differs with the experiment. It indicates that the CC correlation is essential to determine the transition energy, i.e. the wavelength of M1 transition between the multiplets of W^{26+} ions.

The total number of nine M1 or E2 transition in the wavelength range 360-750 nm are illustrated in Fig 2. There are the photo-emission lines which could be observed experimentally. Another two transition are predicted to the most observable M1 transition lines which corresponding to $^3H_6 \rightarrow {}^3H_5$ (467.79nm) and $^3F_3 \rightarrow {}^3F_2$ (501.80nm). These predications have been verified by a new experiment which observed two lines in 464.41 nm and 501.99 nm[2].

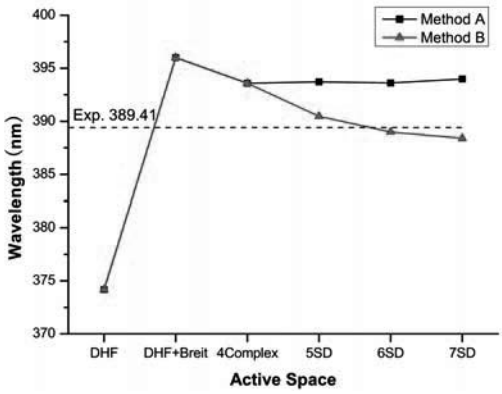

Fig. 1 The wavelength of the M1 transition from the level $^3H_5$ to $^3H_4$ between the multiplets of the ground state $4f^2$ of W^{26+} ions. The Breit interaction effect is included in all calculations except DHF. The horizontal broken line with label 'Exp.' represents the EBIT experiment observation (389.41 nm).

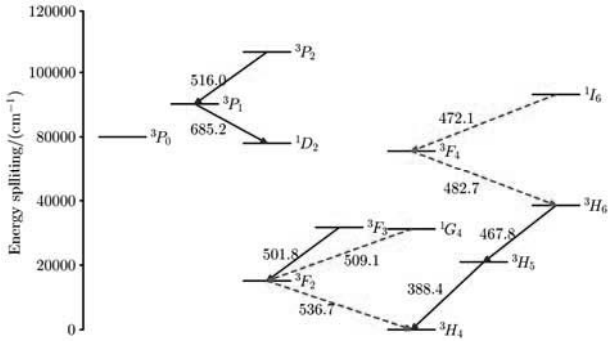

Fig. 2 The energy level and transition diagram of M1 (blue solid) and E2 (read dashed) transition between two connected levels. The highest level $^1S_0$ is omitted from the figure because the level energy is too high to give visible light transitions.

1) Jonsson, P. et.al.:*Comput. Phys. Commun.*,**177** (2007) 597.
2) Ding X.B. et al.: *J. Phys.B* , 44 (2011) 145004.