Preliminary ab-initio calculations of the mean excitation energy of ions with relativistic effects for deriving their stopping power in fusion plasmas

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The use of tungsten as a material for plasma-facing components introduced new challenges for plasma simulation codes. High-Z impurities like tungsten (Z = 74) are not fully ionized in tokamak plasmas in existing devices, nor in the planned ones like ITER or DEMO. Bound electrons strongly influence collisions in different ways, e.g. by introducing new energy loss mechanism by excitation and ionization [1,2].
The effects of impurities on suprathermal electrons dynamics can be calculated using the Fokker-Planck equation with modifications [3] to the collision operator. However, this approach requires knowledge of the Mean Excitation Energy (MEE) of the ions, which precise value can only be obtained from the spectroscopic properties of the ions. Since direct measurements of the required quantities for ions are not possible, the only way to obtain accurate estimates of the MEE is to calculate the transition properties of the ions. This has already been done in non-relativistic approach, but high-Z elements require advanced atomic models that account for relativistic and correlation effects in atoms. Modern computational methods, such as Multiconfigurational Dirac-Hartree-Fock, brings the possibility to obtain required data from ab-initio calculations of atomic properties. Since tungsten is an important element for the spectroscopy of the tokamak plasma, calculations of some tungsten lines are already available [4]. However, no systematic study to obtain the MEE has been done. The presented work shows possible ways to fill this gap and preliminary results of the MEE calculation for ions where relativistic effects are noticeable.

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