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Invited Lecture

AB INITIO AND SEMI-EMPIRICAL ATOMIC STRUCTURE CALCULATIONS. APPLICATIONS TO THE 5s-6p TRANSITIONS FOR THE Mo II ION

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In this work, we present two different methods for calculating atomic structure for atoms and ions.

The first one is the Hartree-Fock pseudo-Relativistic (HFR) method which can be *ab initio* where we calculate the atomic parameters theoretically by using for example the first three programs of the Cowan (CW) atomic structure code: RCN, RCN2 and RCG. We can also use it semi-empirically by using the forth CW program RCE and fitting the purely theoretical energy levels with experimental data taken for example from the NIST database.

The second one is the Thomas-Fermi-Dirac-Amaldi (TFDA) method which can be *ab initio* where we calculate the atomic parameters theoretically by using for example the SUPERSTUCTURE (SS) or the AUTOSTRUCTURE (AS) atomic structure codes. We can also use it semi-empirically by using the Term Energy Corrections (TEC) in SS or the Level Energy Corrections (LEC) in SS or AS atomic structure codes.

As an applications of using these methods, we calculate energy levels, oscillator strengths and transition probabilities for the 5s-6p transitions for the Mo II ion using *ab initio* and semi-empirical methods with the CW and AS atomic structure codes.