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Atomic Calculations and Data Using the MultiConfiguration Dirac-Fock General Matrix Elements (MCDFGME) code

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The current accuracy of atomic calculations is impressive, allowing us to explain and probe novel and extremely rich physical phenomena. In turn, novel experiments constantly allow us to validate and adjust our theories and calculations. The atomic data we can calculate encompasses many physical interactions, providing a wide range of fields with the necessary data for their own studies.
The theory is there for us to use, however we must apply it in a practical manner for a variety of bound systems, which oftentimes require hundreds of thousands of separate calculations. This brings the question of how are we going to, in a more practical and autonomous manner, implement our theories to produce usable atomic data?
In this talk I will show you how we currently utilize the MCDFGME code [1] to perform atomic calculations on a variety of atomic systems and obtain useful, reliable and accurate atomic data. I will also bring attention to a few details of the calculation method which, if not considered, could result in erroneous calculations and atomic data. Finally, I will show you recent atomic data that we have calculated using this code, which can also be obtained experimentally.

References:
[1] J. P. Desclaux, A multiconfiguration relativistic DIRAC-FOCK program, Computer Physics Com-munications 9 (1) (1975) 31–45. doi:10.1016/0010-4655(75)90054-5.

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