Abstract Submitted
for the DAMOP15 Meeting of
The American Physical Society

Large-scale relativistic calculations of ionization energies and total binding energies of all atoms and positive atomic ions with nuclear charge Z = 1-110 ALEXANDER KRAMIDA, CHARLOTTE FROESE FISCHER, JOSEPH READER, National Institute of Standards and Technology, PAUL INDELICATO, Laboratoire Kastler Brossel, Ecole Normale Superieure, CNRS, Sorbonne Universites, France — The latest versions of advanced multiconfiguration Dirac-Fock atomic codes, MCDFGME and Grasp2K, are used to calculate ionization energies (IE) and total binding energies of all atomic systems. Comparison with experiment and other benchmark data shows an excellent accuracy achieved in these calculations for H-, He-, and Li-like ions. In particular, our results for H-like ions with Z >2, obtained with the MCDFGME code, are the most accurate available today. For multi-electron ions, we combine the accurate single-configuration MCDFGME calculations with the correlation-difference energy (difference between the multiconfiguration and single-configuration total energies) calculated with Grasp2K. This approach results in a dramatically improved agreement of calculated IEs with experiment (less than 0.7 eV on average) for all systems, excluding those involving open f-shells. The most probable ground states are found for most systems, leaving questionable only about 100 out of total 6105 considered systems.

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Date submitted: 30 Jan 2015 Electronic form version 1.4