

# Accuracy in atomic and molecular data

Gordon W. F. Drake

*Department of Physics, University of Windsor, Windsor, ON N9B 3P4 Canada*

As undergraduates we all learned how to estimate the uncertainties in experimental measurements, and error bars are a standard part of published results. However traditionally the same has not been true on the theoretical side. There has long been a tendency to publish theoretical calculations without uncertainty estimates, or even an indication of how many figures are significant. This limits the usefulness of the results in comparing with experiment (do they agree or not?) or in applications to other areas such as astrophysics or plasma modeling. The situation is now changing with advances in techniques for estimating uncertainties, and requirements for uncertainty estimates in published data [1, 2]. The talk will focus on sources of uncertainty in calculated atomic and molecular data involving atomic and molecular structures and cross sections for electron-atom, electron-molecule, and heavy particle collisions. Following a recent review article [3], the talk will discuss model uncertainties due to approximations to the fundamental many-body quantum mechanical equations with the aim of providing guidelines to estimate uncertainties as a routine part of computations of data for structure and scattering.

- [1] Drake GWF 2010 "Role of accuracy estimates in atomic and molecular theory" in *Proc. 7th Int. Conf. on Atomic and Molecular Data and their Applications - ICAMDATA-2010* Edited by Bernotas A, Karazija R and Rudzikas Z *AIP Conf. Proc.* 1344 pp. 9–24
- [2] The Editors 2011 *Phys. Rev. A* **83** 040001
- [3] Chung HK, Braams BJ, Bartschat K, Csaszar AG, Drake GWF, Kirchner T, Kokoouline V and Tennyson J 2016 *J. Phys. D–Appl. Phys.* **49** 363002