Group discussion:
Accurate and comprehensive collision data sets and their uncertainties

Editorial: Uncertainty Estimates, Physical Review A 83, 040001 (2011)

Joint IAEA-ITAMP Technical Meeting on the Uncertainty Assessment for Theoretical Atomic and Molecular Scattering Data, Cambridge, MA, USA during 7-9 July 2014
https://www-amdis.iaea.org/meetings/ITAMP/

Topical Review: Uncertainty estimates for theoretical atomic and molecular data, H-K Chung *et al* 2016 *J. Phys. D: Appl. Phys.* **49** 363002

Error estimates of theoretical models: a guide, J Dobaczewski, W Nazarewicz, P-G Reinhard, J. Phys. G: Nucl. Part. Phys. 41 (2014) 074001

Collision data sets:
open source, freely available – available in free databases LXCAT, your own sites, institutional sites…

Experiment & Theory
Experiment
can be accurate, but unlikely comprehensive,
very important for model verification & testing: crucial for work on complex atoms & molecules
relatively standard error estimation
major problem: less and less active exp. groups… are there ways to change it? funding…

Theory
often the only way to get the data: radicals, isotopologues, excited states…
can be both: accurate and comprehensive: but likely only for simple systems,
very different for complex systems (tungsten, complex molecules…) – hard to estimate accuracy, too many reaction channels - are there ways to deal with it?

Accurate & comprehensive
Priorities…
Comprehensive:
Full datasets are often required: all ionization stages, across low to high energies, etc…
What datasets/ databases are available?
Strategies for adoption / advertisement of new accurate datasets.
Do we want to move to the "recommended" database?

Accuracy / uncertainties: where the errors come from?
Missing physics, poor description of the system, truncation effects…
Uncertainties: random or systematic

Fundamental atomic data and derived atomic data

What atomic data are important? Depends on the application…
How sensitive are the simulations to atomic physics? ← likely this is the crucial consideration
Link to and across communities for both points

Techniques for uncertainty quantification: least square, Monte-Carlo, ...
Shall we produce/recommend a specific rule-set for the collision data producers to follow?

Techniques to conduct collision calculations: close-coupling (R-matrix, CCC, TDCC….), ECS, DW, FBA, BEB,…
Reaction channels: elastic, inelastic, ionization, dissociation, charge exchange,…
Schrodinger or Dirac formulations…