INTERNATIONALLY COORDINATED ACTIVITES ON ASSESSING ATOMIC, MOLECULAR AND PLASMA-SURFACE INTERACTION DATA FOR FUSION APPLICATIONS

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The important objective of the Atomic and Molecular (A+M) Data Unit at IAEA is to provide evaluated and recommended databases on A+M processes and plasma-material interaction (PMI) processes for nuclear fusion and other plasma applications. In recent years, complex and sophisticated data sets for A+M and PMI processes are required for applications and yet available data are predominantly and unavoidably calculated data. For calculated data, however, assessment and evaluation is very difficult. There is no tradition or culture of estimating uncertainties in calculated data and there is no accepted formal procedure for evaluating and recommending such data.

Recently, an editorial standard of Physical Review A requires that certain classes of atomic data must be published with uncertainty information and it specifies that advances in techniques for the evaluation of data and assessment of uncertainties qualify as "new physics" [1]. Therefore the community of calculated A+M data is beginning to recognize that uncertainty quantification (UQ) and critical assessment of theoretical A+M data beyond the simple comparison with measured data is an independent and worthwhile scientific interest.

The A+M Data Unit has collaborated with A+M community to develop guidelines for critically assessing theoretical atomic and molecular structure and collision data, taking into account the processes and the quantity of interest as well as specific theoretical methods employed in calculations. Recently, the Unit also began to collaborate with researches in the PMI fields of electronic structure calculations, molecular dynamics and multi-scale modeling to address UQ issues. The progress towards guidelines for evaluation of theoretical A+M collision data and internationally coordinated activities at IAEA towards the UQ sciences of A+M/PMI data will be reviewed.

References

[1] Editorial in Phys. Rev. A 83, 040001 (2011).