

Uncertainty evaluation in theoretical calculations of cross sections for electron-molecule collisions

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In this talk, two approaches for uncertainty assessment in theoretical calculations of cross sections for electron-molecule and atomic collisions will be discussed. In particular, a systematic Monte-Carlo approach, used in nuclear physics, for the uncertainty quantification will be reviewed and presented in the framework of electron-molecule collisions. The approach allows one to evaluate the uncertainty of final theoretical cross sections if uncertainties of all parameters used in the model are available. It can also deal with parameters of the theoretical model that are correlated. Correlations between parameters often reduce uncertainties of final results and, therefore, should be accounted for if data of a high value is under consideration. The approach allows also a systematic comparison with experimental data (if they are available). The procedure gives a standardized way to produce evaluated (recommended) cross sections and uncertainties combining information from different theoretical and experimental sources.

*This work is partially supported by the National Science Foundation, Grant No PHY-15-06391.