

PiAI Seminar Series: Physics informed AI in Plasma Science
7:00-8:00, 22 April 2024 (CDT)
14:00-15:00, 22 April 2024 (CEST)
21:00-22:00, 22 April 2024 (JST)
Web Seminar

**A Machine Learning Model for Estimating Electron- and Proton-
Impact Collision Cross Sections**

Allison Harris

Illinois State University Physics, IL, USA

Charged particle collision cross sections play an important role in many areas of applied physics, but detailed measurements and state-of-the-art theoretical calculations are often too difficult or expensive to perform for highly complex molecules or for a wide variety of atomic and molecular targets and collision energies. Consequently, the needed data sets are often unavailable or incomplete. Machine learning algorithms may be able to provide reasonable estimates for atomic and molecular targets that are beyond the reach of theoretical models and experimental measurements and help fill the gap in available cross section data. We present results from feed-forward neural networks that were trained on published experimental data and show that they provide reasonable estimates of electron- and proton-impact collision cross sections for atomic and molecular targets beyond those in their training sets. We test our models by comparing their predictions with measured cross sections, and show that with training on as a few as 15 molecular targets, cross sections can be predicted to within 10% for many molecules. The success of our simple models with relatively few training data sets indicates that machine learning algorithms can successfully complement experiment measurements and traditional theoretical models and are a viable alternative to provide much needed data for applied physics modeling.