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A machine learning based model for predicting molecular ionization cross sections[1] LINLIN ZHONG, School of Electrical Engineering, Southeast University, No 2 Sipailou, Nanjing, Jiangsu Province 210096, P. R. China — The electron-impact ionization of molecules is one of the most fundamental collision processes in plasma physics as well as in many areas of application. The electron-impact ionization cross section of a molecule is the key parameter of describing electron-molecule collision ionization. Since obtaining ionization cross sections through experiments is very expensive in most cases, many efforts have been devoted to their theoretical determination. However, the theoretical calculation of molecular ionization cross sections requires the *ab initio* computation which is time-consuming especially for large molecules. Recently, we propose a data-driven model based on machine learning to fast predict molecular ionization cross sections. This model is learned from the data of the small molecules which have less constituent atoms than the large molecule we study. Any machine learning algorithms, such as support vector machine (SVM), can be used to train the model. Our tests indicate that this machine learning based model can generate well-agreed ionization cross sections of molecules and has good generalization performance.

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