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Extensible Algorithmic Generation of Molecular Electron-Impact Cross-Section Data from DFT Information for Simple Organic Molecules[1]

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— Medical and industrial atmospheric pressure plasma discharges frequently involve complex electrochemical reaction networks with large organic molecules. Modeling of these networks which may contain thousands of species and hundreds of thousands of reactions is infeasible by manual methods, and so must be handled algorithmically. In this work, a preliminary software framework for handling large plasma-chemistry problems is presented. The framework currently generates usable electron-impact cross-section datasets for species within the reaction network using the open-source DFT software NWChem, and automatically assembles the corresponding plasma-chemistry network using the CRANE (https://github.com/lcpp-org/crane) open-source software. We show an example on how to create a reaction network for ethylene, a small well-studied organic molecule, and extend the same algorithmic approach to isopropyl alcohol. Comparisons to experimental cross-sections and prior computational work on ethylene is discussed. We also explore computational scaling to larger molecules and reaction networks, including the effects of adding additional reaction mechanisms or levels of theory.

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