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Semi-Classical Reaction Network Generation from Localized Molecular Orbital DFT for Arbitrary Network Complexities STEVEN MARCINKO, DAVIDE CURRELI, University of Illinois at Urbana-Champaign — When modeling atmospheric-pressure plasma sources, one of the main challenges is on the construction of the reaction network describing the plasma chemistry of the system. Reaction network size scales exponentially with the number of atom identities and molecular bonds in the network precursors, prohibiting time-intensive multivariate transition state calculations to find branching ratios for dissociative processes. The size of the network alone may be too large to handle, with 10^6-10^9 or more potential reactions for large precursor molecules. In this work we show a method to generate reaction networks using established classical and semi-classical relations, combined with information from ML-assisted localized molecular orbital DFT, including electron-driven excitation, scattering, and dissociation, as well as prominent heavy-species reactions such as de-excitation and charge exchange. We assess accuracy and precision of the method via a comparison of the density and reaction rate outputs of a 0D model from both an automatically-produced and hand-produced network of some common network chemistry (e.g. Ar, He/N, Si/H). Furthermore, we show strategies for complexity mitigation, including runtime application of network reduction strategies on networks from larger precursors.

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