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Electron-driven excitation and dissociation of molecules¹

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Due to the large difference in mass between the electron and the nuclei, when an electron collides with a molecule or molecular ion, there is inefficient transfer of energy from the electron into the motion of the nuclei, leading to little vibrational excitation or dissociation. However, in certain special cases, the electron can temporarily attach to the molecule and change the forces felt between its atoms for a period of time comparable to a vibrational period. This can lead to resonant vibrational excitation and dissociative attachment, for neutral targets, or dissociative recombination in the case of ions. Studies of dissociative recombination and attachment in several polyatomic systems have shown that simple one-dimensional models can fail to capture the correct dissociation dynamics. In our treatment of these processes we first carry out *ab initio* electron scattering calculations at fixed internuclear geometries to determine the resonant energy surfaces and the corresponding surface of autoionization widths using the Complex Kohn variational method. These resonance positions and widths are then used as input to a dynamics study to determine the cross-section and product distributions for the dissociation or excitation process. We will present results on a number of systems, including HCCH, HCN/HNC and HCCCN as examples of dissociative attachment and N_2H^+ and H_2O^+ for dissociative recombination.

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