Understanding the dynamics of chemical bond dissociation under the electron beam: computational perspective

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Chemical bond dissociation is a central concept in Chemistry. Transmission electron microscopy (TEM) has emerged as a tool for triggering bond dissociation in single molecules and materials by harnessing the kinetic energy of fast electrons of the electron beam. The use of the electron beam as a stimulus of chemical reactions and as a sub-angstrom resolution imaging probe allows investigations of the molecular dynamics and reactivity in real time and at the atomic scale. The dynamics of chemical bond dissociation can be also probed indirectly by vibrational electron energy loss spectroscopy in situ during scanning TEM experiments. In this talk, we will explain how the electron beam can trigger homolytic dissociation of the H–F or H–O bonds inside fullerene cage, leading to entrapment of F and O atoms, and discuss knock-on mechanisms of bond dissociation and atom permeation through C60. [1] A separate example of knock-on damage will be introduced in the context of understanding the electron stability of two-dimensional conjugated metal organic frameworks (thin films) which exhibit complex damage mechanisms with non-trivial fragmentation pathways. [2]

[1] J. Biskupek et al., *ACS Nano* **14**, 11178 (2020).
[2] Mücke, D. et al., *Nano Letters* **24**, 3014 (2024).