Bond-selective reactions observed during molecular collisions

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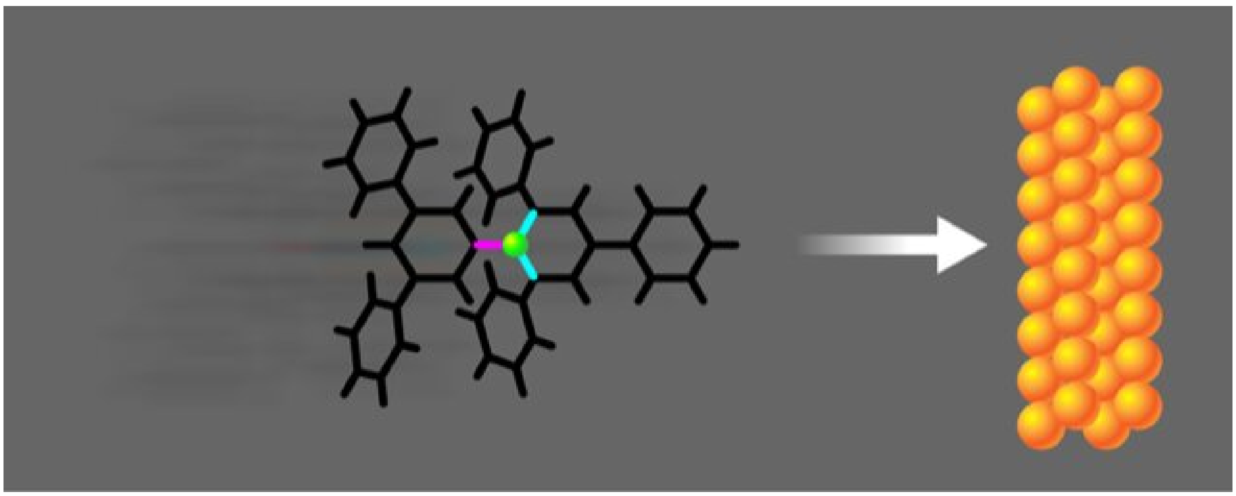

A Reichardt's dye molecule colliding at hyperthermal velocity with a copper surface. The molecule's orientation determines whether the energy of the collision is concentrated in one of the bonds between the central nitrogen atom (green) and a carbon atom in one of the surrounding rings (black). Credit: L. Krumbein et al. ; adapted by APS/Alan Stonebraker

A team of researchers from Germany and the U.K. has found that bond-selective reactions can be observed during certain molecular collisions. In their paper published in the journal *Physical Review Letters*, the group describes experiments they conducted that involved firing a large molecule at a wall of copper and what they discovered by doing so.

Over the past several decades, chemists have been looking for a way to break specific bonds in molecules in a predictable and usable way. Doing so would open up new avenues of research involved in creating new kinds of compounds. Such efforts have by stymied, however, by the way that energy is dissipated in molecules. When a laser is fired at a molecule, for example, its energy is dissipated through vibrations before a reaction can occur. The end result is virtually identical to simply applying heat to the same molecule. In this new effort, the researchers have found a way to conduct bond-selective reactions by firing molecules at a copper wall.

In their experiments, the researchers used a type of molecule known as Reichardt's dye—a large (73 atom) molecule that changes color depending on the type of solvent used in a reaction. They fired single instances of the molecule at a piece of flat copper crystal and watched what happened using a scanning tunneling microscope.

The researchers found that the Reichardt's dye molecule underwent profound changes as it slammed into the copper wall, while the wall remained completely intact. The collisions were reminiscent of cars slamming into walls for safety tests. In studying the collisions, the researchers found that when the molecule collided with the wall at certain translational energies, the molecule would experience selective cracks at specific C-N bonds. Cracking meant that some of the bonds in the molecule would break but the molecule would remain as a single entity. They also found that changing the speed at which the molecule was fired at the wall allowed them to break two specific bonds, which happened to be adjacent to a positively charged nitrogen atom sitting at the center of the molecule.

More work is required to determine if the new approach can be applied in useful ways—but for now, the team describes selective bond chemistry as "less of a black box" now.

More information: Lukas Krumbein et al. Fast Molecular Compression by a Hyperthermal Collision Gives Bond-Selective Mechanochemistry, *Physical Review Letters* (2021). DOI: 10.1103/PhysRevLett.126.056001 . On *Arxiv*: arxiv.org/abs/2007.04497