Molecular dance that could eliminate soot pollution

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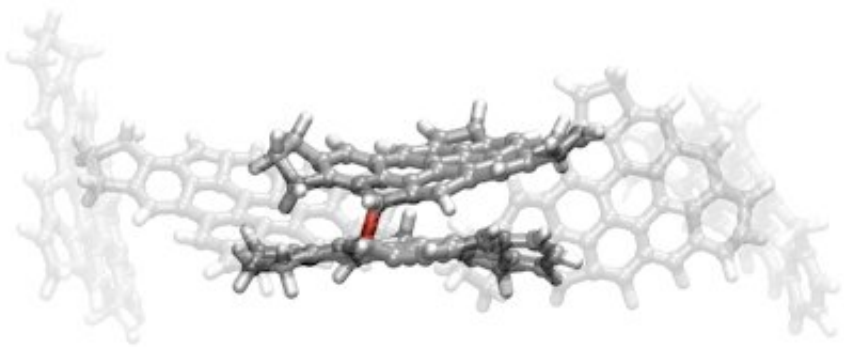

Reactive dimerisation of pi-diradicals. Credit: Jacob Martin

A hidden, newly discovered molecular dance could hold the answer to the problem of soot pollution.

Soot pollution causes cancer and blood clots, as well as weakening immune systems to respiratory viruses. The atmosphere and glaciers are also blanketed by soot, leading to global heating and increased ice loss. Surprisingly, the way that soot particles form is still unknown, but is of pressing concern

The reason for this long-running mystery is due to the extreme environment in which soot forms, the rapid speed of the reactions and

the complex collection of molecules present in the flame. All of these obscure the pathway to soot formation.

An international team from the UK, Singapore, Switzerland and Italy has now used two microscopes to reveal the molecules and reactions taking place in a flame. The first microscope operates by touch, feeling for the arrangement of atoms in the molecules of soot. These tactile maps provide the first picture of soot's molecular chicken wire shape. Quantum chemistry was then used to show that one of the molecules was a reactive diradical. A diradical is a type of molecule with two reactive sites, allowing it to undergo a succession of chain reactions.

The second microscope is entirely virtual and shows the reaction between the diradicals. Quantum mechanics guided a supercomputer to virtually and realistically collide the molecules together and reveal the molecular dance in slow motion.

This simulation showed that the individual molecules are held together by intermolecular forces after they collide. This gives the reactive sites time to find each other and create a permanent chemical bond. Even after they have bonded they remain reactive, allowing more molecules to "stick" to what is now a rapidly growing soot particle.

This discovery could resolve the problems with previous attempts to explain soot formation via either a physical condensation or chemical reaction. In fact, both are required to adequately explain the rapid and high-temperature reactions.

One of the paper's lead authors, Jacob Martin, said, "If the concentration of these species is high enough in flames, this pathway could provide an explanation for the rapid formation of soot."

Co-author Markus Kraft, from the University of Cambridge's

Department of Chemical Engineering and Biotechnology, said, "The project brought together cutting-edge computational modeling and experiments to reveal a completely new reaction pathway which potentially explains how soot is formed. Scientists and engineers have been working on solving this important problem for decades."

The researchers hope to target these reactive sites to see whether the soot formation process can be halted in its tracks. One promising option is the injection of ozone into a flame, which has already been found to effectively eliminate soot in some preliminary results in other work.

"Diradical aromatic soot precursors in flames" is published in *Journal of the American Chemical Society*.

More information: Jacob W. Martin et al, π-Diradical Aromatic Soot Precursors in Flames, *Journal of the American Chemical Society* (2021). DOI: 10.1021/jacs.1c05030

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