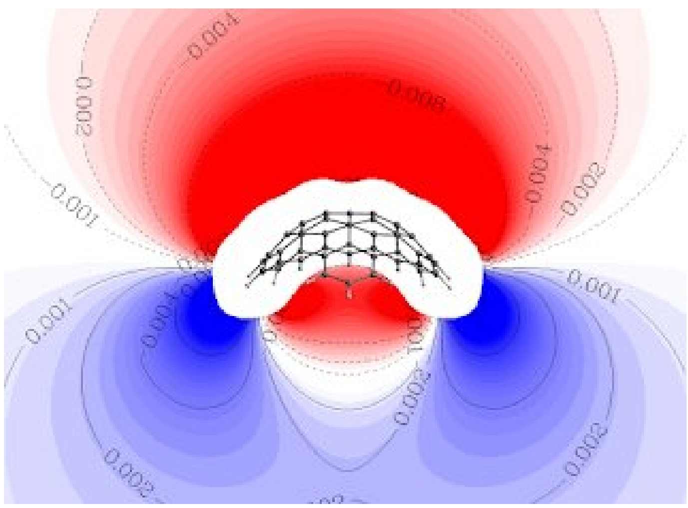
Soot forensics: Carbon fingerprints reveal curved nanostructure

September 19 2018, by Louise Renwick



The electric potential around a curved aromatic molecule. Credit: Jacob Martin

Researchers have moved one step closer to reducing air pollution from engines by imaging soot nanoparticles to reveal their unique signatures. The nanoparticle structures are like fingerprints, revealing curved fullerene-like molecules and helping to shed light on the earliest stages of soot formation.

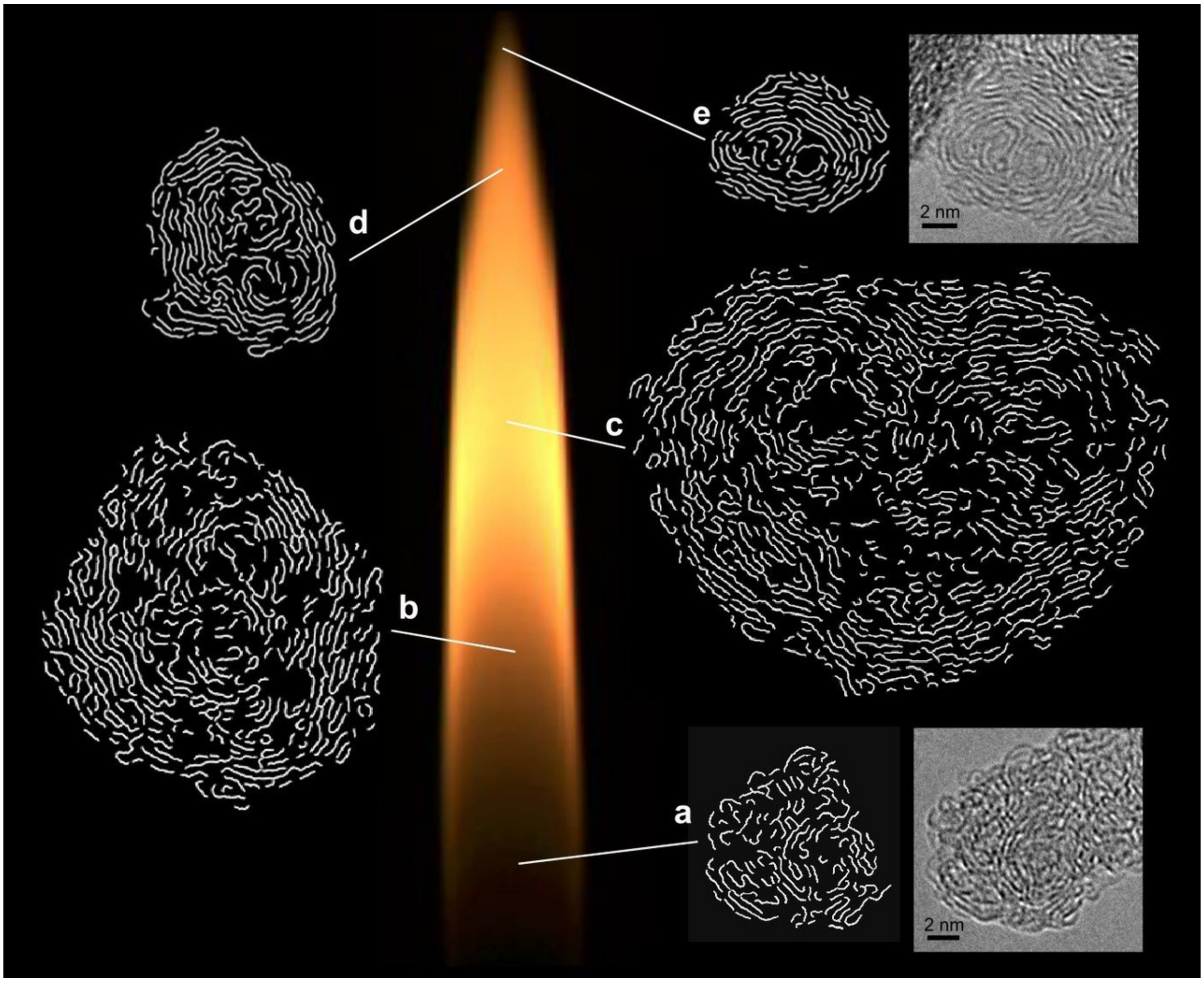
Soot makes up a large proportion of human pollution, clogging our engines and lungs. Soot also contributes to heating the atmosphere while airborne and warming ice once settled, damaging the planet.

Understanding how to stop soot formation in engines presents a unique opportunity to rapidly reduce warming, increase air quality and improve engine efficiency. However, achieving this has been challenging due to the speed and complexity of the chemical reactions involved.

In a recent publication, researchers from the University of Cambridge, National University of Singapore and Nanyang Technological University used an electron beam to image the carbon-rich, saucer shaped molecules that make up soot. Each dark fringe, which corresponds to one of these saucers imaged side-on, was analyzed. Interestingly, they found that these early soot nanoparticles contain many curved molecules, indicating pentagon integration into the normally hexagonal arrangement of carbon atoms. The majority of fringes (>62.5 percent) indicated pentagon-induced curvature in the earliest soot particles.

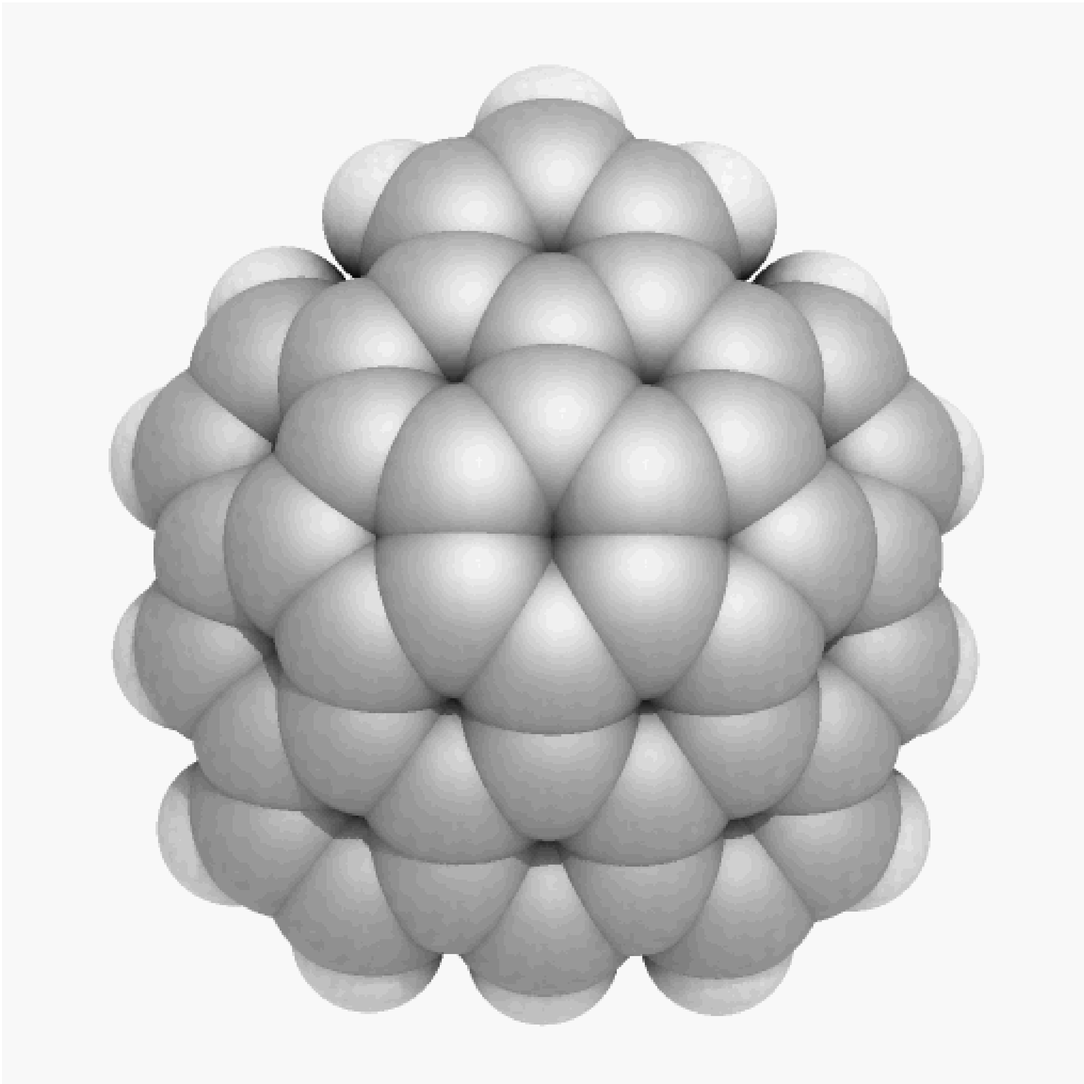
Any aromatic curved by pentagon integration will contain a large charge polarization. The flexing of the molecule causes a charge imbalance on the two faces leading to a permanent dipole moment – the flexoelectric effect. Taking an aromatic molecule, which matches that suggested from microscope images, a significant dipole moment two to three times that of water was found.

These polar species are suggested to impact soot formation through strong interactions with charged species that are produced in abundance in flames. Binding energies were calculated to be sufficient to be able to stabilize small clusters of polar aromatic molecules around these chemi-ions.



Soot fingerprints from electron microscopy reveal curved molecules in early soot particles. Credit: Jacob Martin

This suggested mechanism explains many observations, such as the ability of electric fields to halt soot formation and the similar concentration of chemi-ions to soot nanoparticles. This also provides a new route to reduce soot pollution from engines by either reducing the curvature of the aromatics as they grow or removing the charged species using electric fields.



Model of curved aromatic molecule suggested by electron microscopy. Credit: Jacob Martin

More information: Jacob W. Martin et al. Flexoelectricity and the Formation of Carbon Nanoparticles in Flames, *The Journal of Physical Chemistry C* (2018). DOI: 10.1021/acs.jpcc.8b08264

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