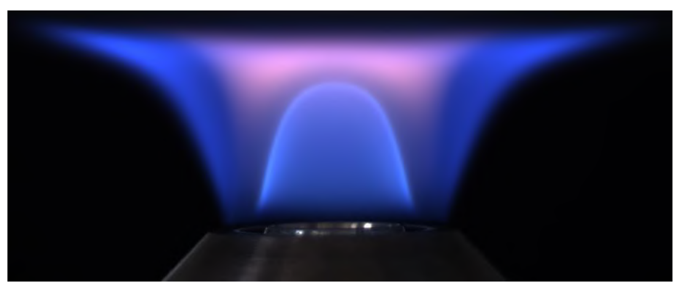
JOINT FINAL EVENT

PaREGEn + PEMs 4Nano

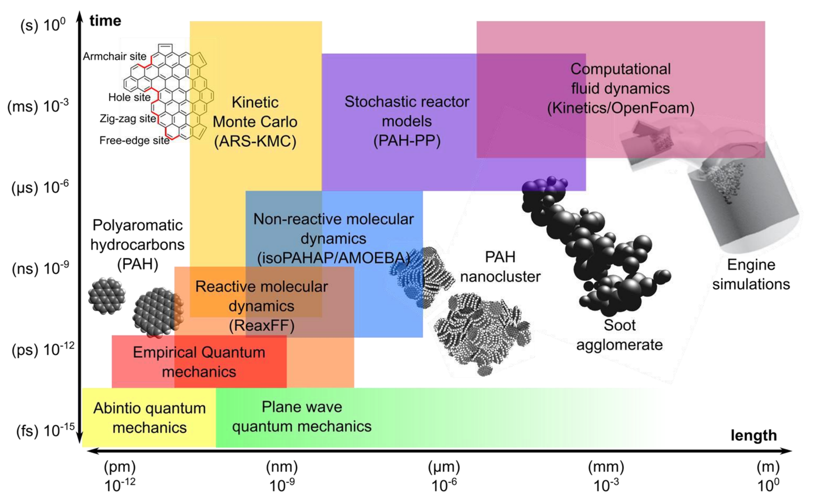
Understanding the Multiscale Formation of Soot



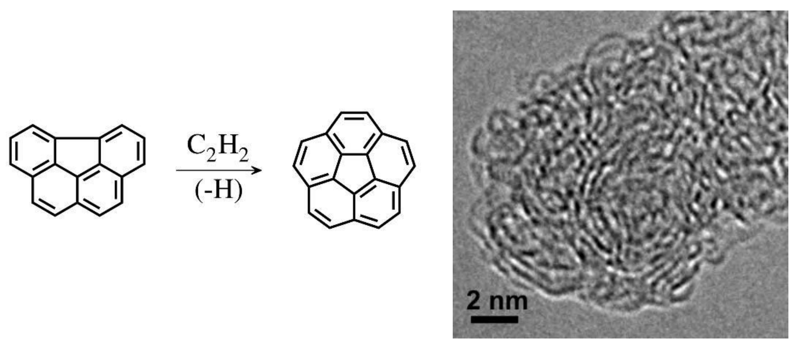
This work presents the advances we have made on the multiscale understanding of soot formation. Insights into the presence of curved polar aromatics, detailed modelling, mechanical properties and biofuels are highlighted

Soot reduction at all scales

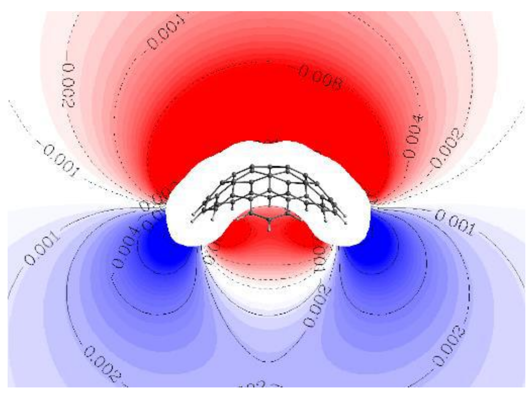
Soot contributes to climate change and causes an estimated 7 million premature deaths p.a. We seek to reduce soot emissions by understanding the processes responsible for its formation.



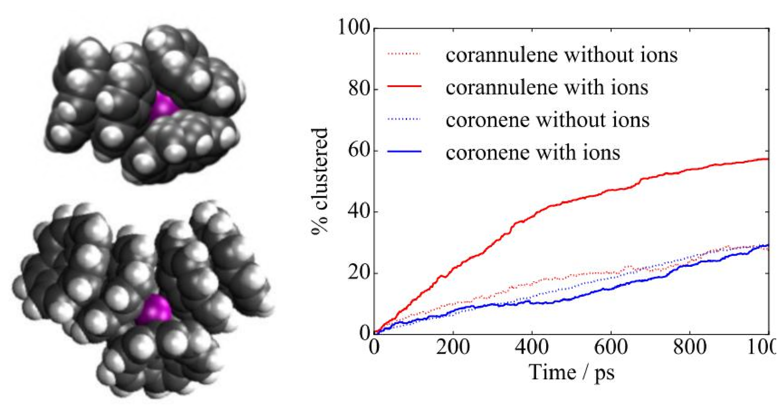
Polar aromatics in soot



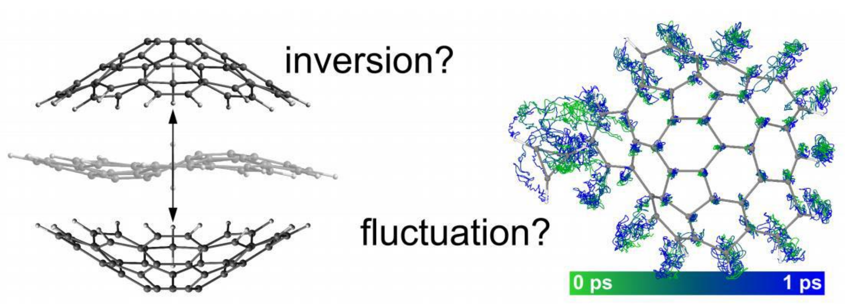
Electron microscopy shows evidence for the existence of curved species in soot particles.



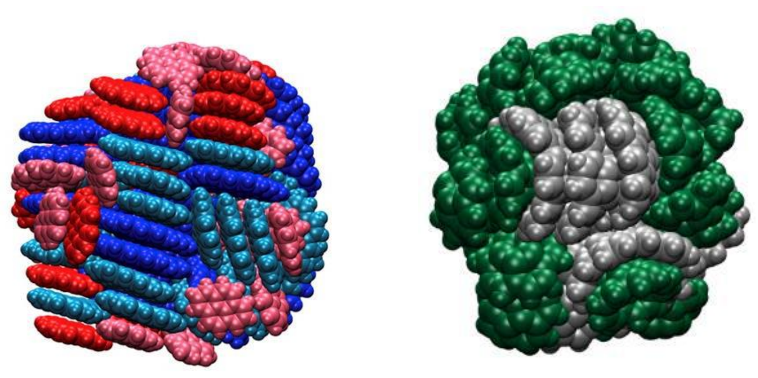
Curvature causes a large electric polarisation, roughly two to three times that of water.



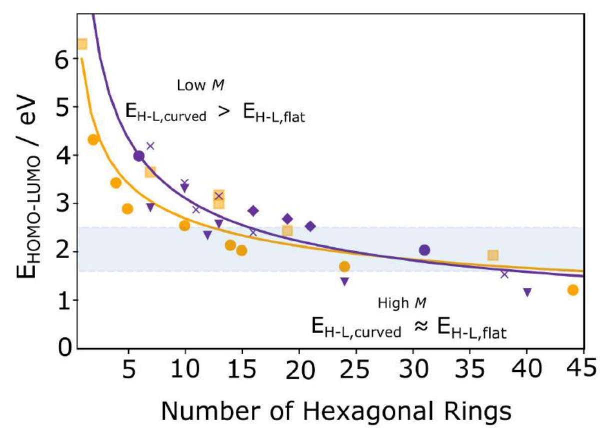
Simulations show that the electric polarisation can cause curved species to cluster around ions.



The electric polarisation was shown to persist at flame temperatures for modest sized species.

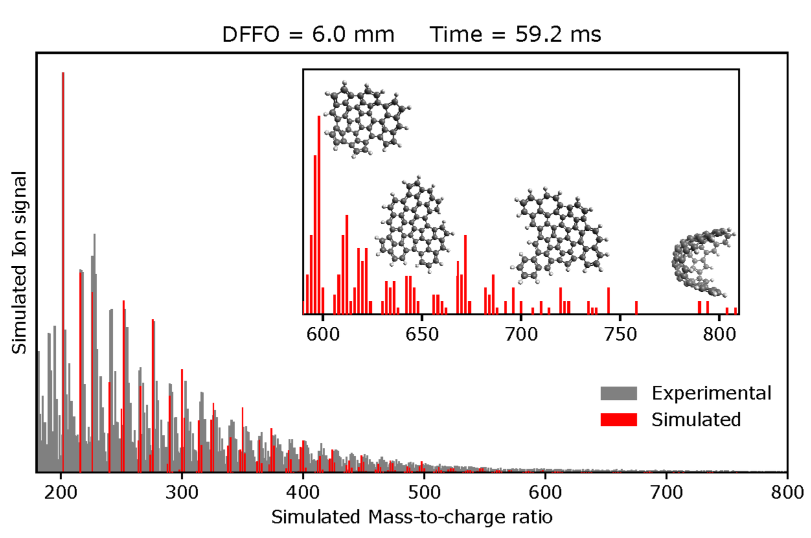


Heterogeneous particles containing curved and flat species of different sizes show distinct properties.

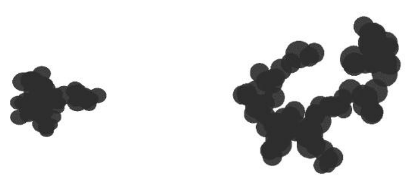


The impact of curvature on the optical band gap has been computed to help interpret diagnostic data.

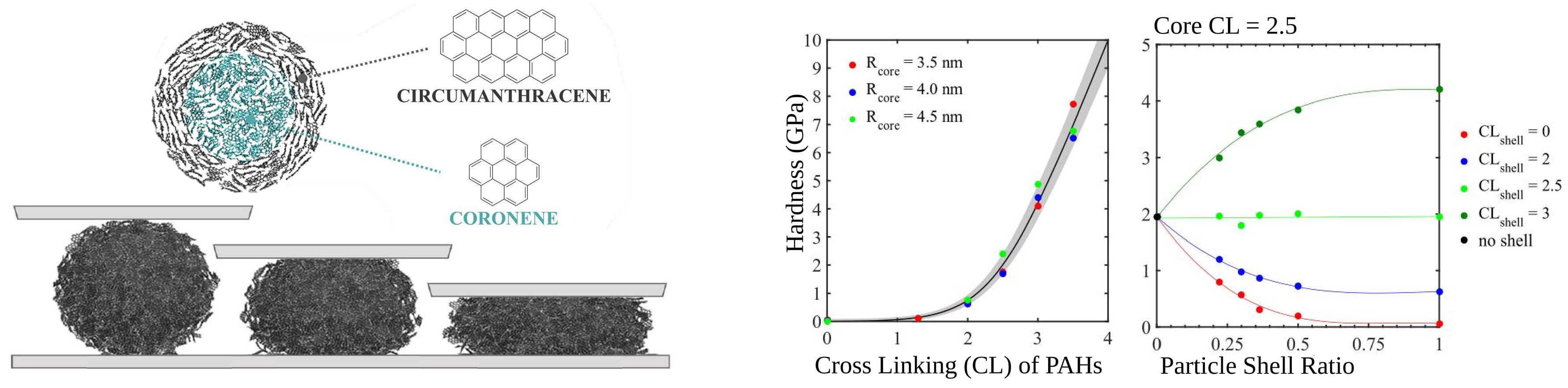
Detailed models for soot formation



A detailed population balance model allows direct comparison of simulations with experimental data, for example mass spectra and images from transmission electron microscopy.

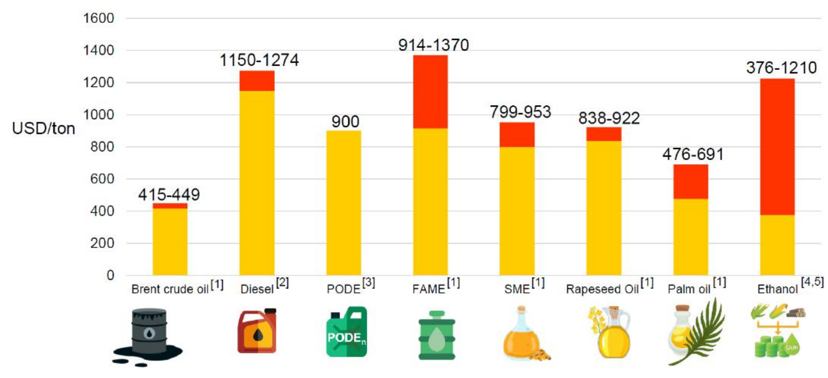


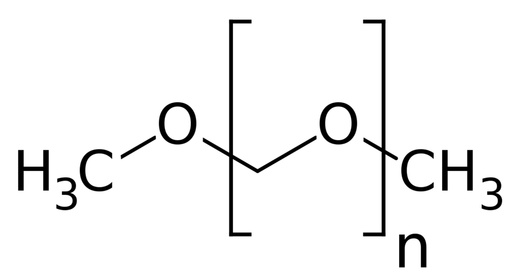
Soot hardness indicates crosslinks



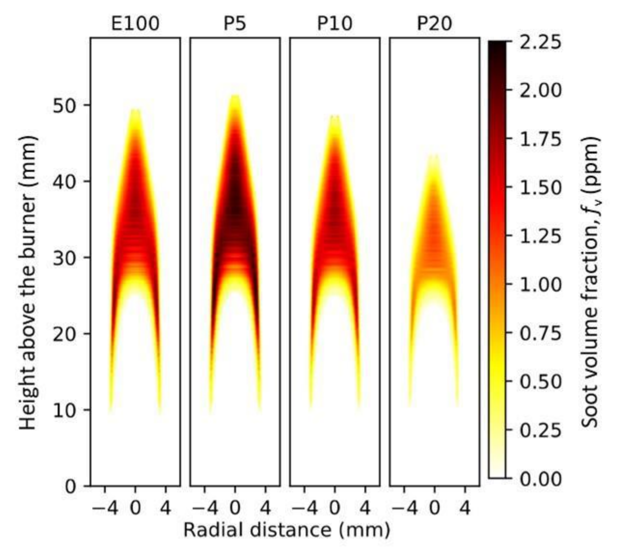
Simulation of the nanoindentation of soot allows the calculation of the mechanical properties as a function of the internal structure of the particles. Comparison with experimental data provides insight into the number and type of bonds between the molecules in the particle.

Biofuels and oxygenated fuels

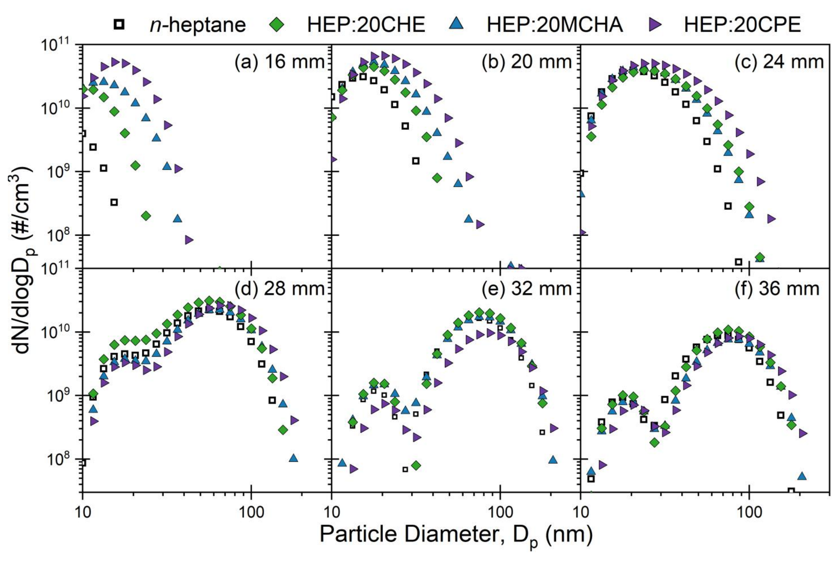




Polyoxymethylene dimethyl ethers (PODE) are being investigated as potential biofuels and as a means to reduce particulate emissions. PODE are interesting because they contain no C—C bonds.



Doping a flame with more than 10% (by carbon) $PODE_3$ reduces the amount of soot formed in the flame.



The presence of cyclic fuels promotes particle formation due to enhanced growth of aromatic species.

Acknowledgements and further information

CoMo Group Website | https://www.como.ceb.cam.ac.uk

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