

Surface properties of heterogeneous polycyclic aromatic hydrocarbon clusters

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The team



Kimberly
Bowal

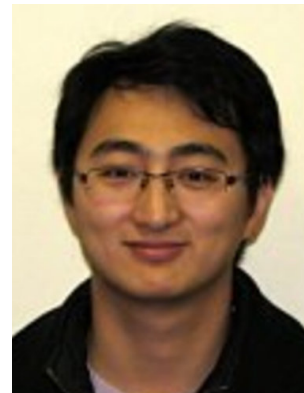


Laura
Pascazio



Hongyu
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Institute of
Technology



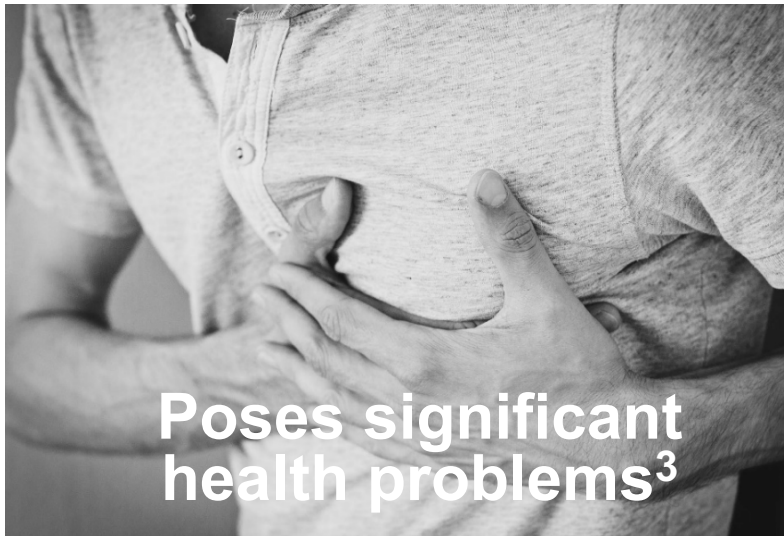
Dongping
Chen

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Technology



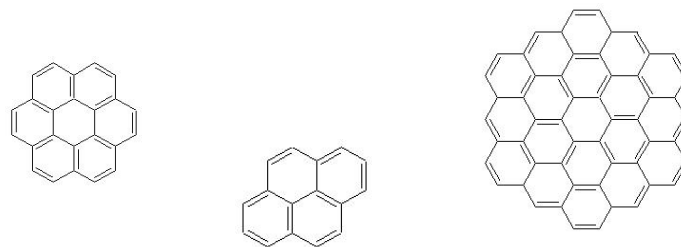
Markus
Kraft

Why study soot?



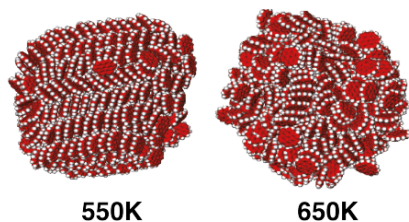
Soot particle model

Detailed atomic studies of soot particles examine clusters containing polycyclic aromatic hydrocarbons (PAHs)



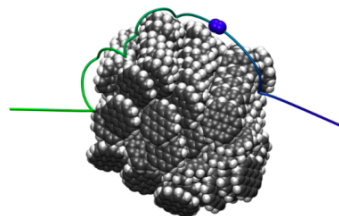
Melting behaviour

Chen, D. et al. Carbon, 67 (2014)



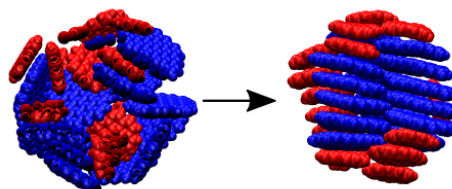
Interactions with gaseous species

Grancic, P. et al. Carbon, 109 (2016)



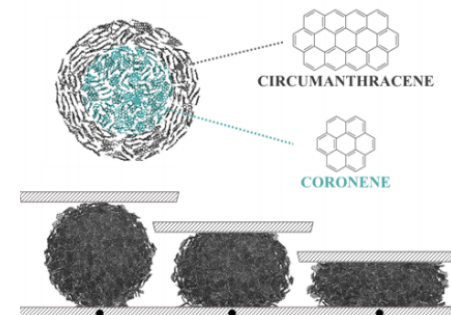
Molecule self-assembly

Bowal, K. et al. Carbon, 143 (2019)



Particle hardness

Pascazio, L. et al. Combust. Flame 219 (2020)



Aim: Use molecular modelling methods to provide a detailed numerical evaluation of soot particle surface properties

Simulation methods

- Varying particle size, molecule size, molecular ratio
- Replica exchange molecular dynamics to obtain particles across a wide range of temperatures
- Solvent-excluded surface analysis to evaluate the particle surfaces
- Reactive sites: hydrogen atom (H), carbon atom (C), internal carbon atom (IC), edge carbon atom (EC), free-edge site (FE), zig-zag site (ZZ)

PYR ($C_{16}H_{10}$)



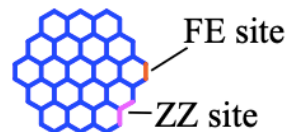
COR ($C_{24}H_{12}$)



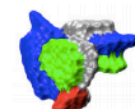
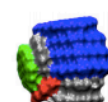
OVA ($C_{32}H_{14}$)



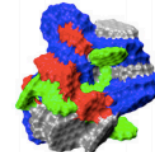
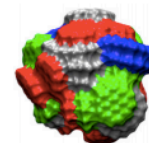
CIR ($C_{54}H_{18}$)



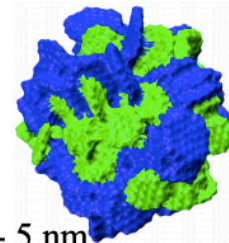
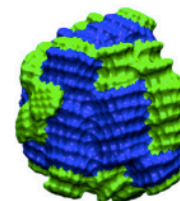
Low temperature High temperature



Quaternary (nonuniform) - 2 nm



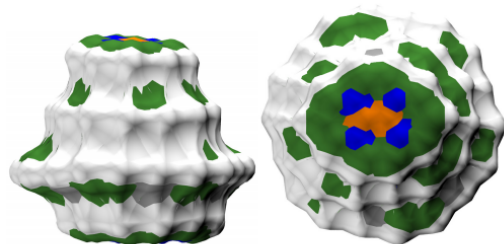
Quaternary (uniform) - 3 nm



Binary - 5 nm

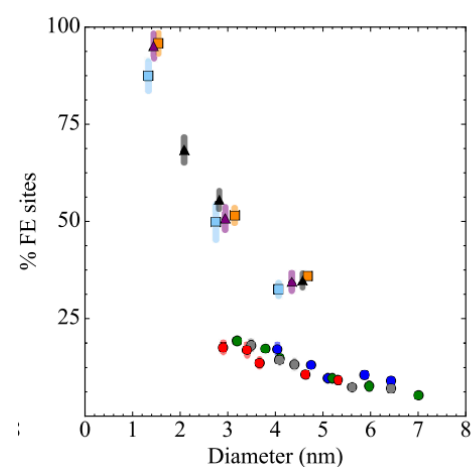
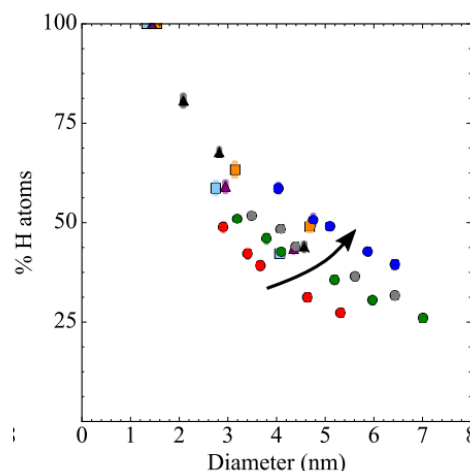
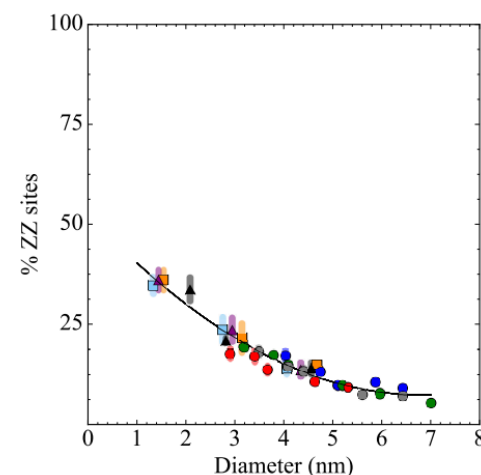
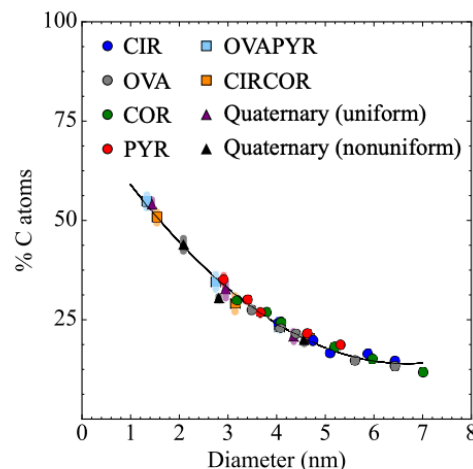
Percent on surface

- % of C atoms and ZZ sites on surface not dependent on particle composition
- % of H atoms on surface related to constituent molecule sizes
- % of FE sites on surface dependent on molecular heterogeneity

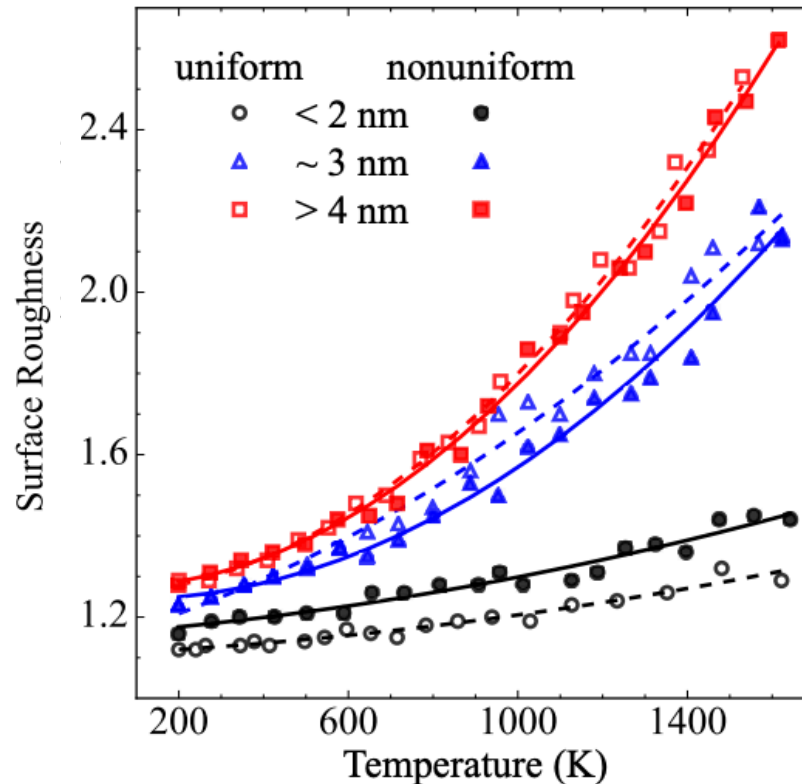


(a) Side view

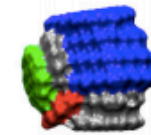
(b) Top view



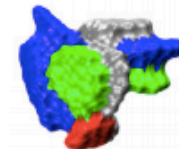
Particle roughness



Low temperature

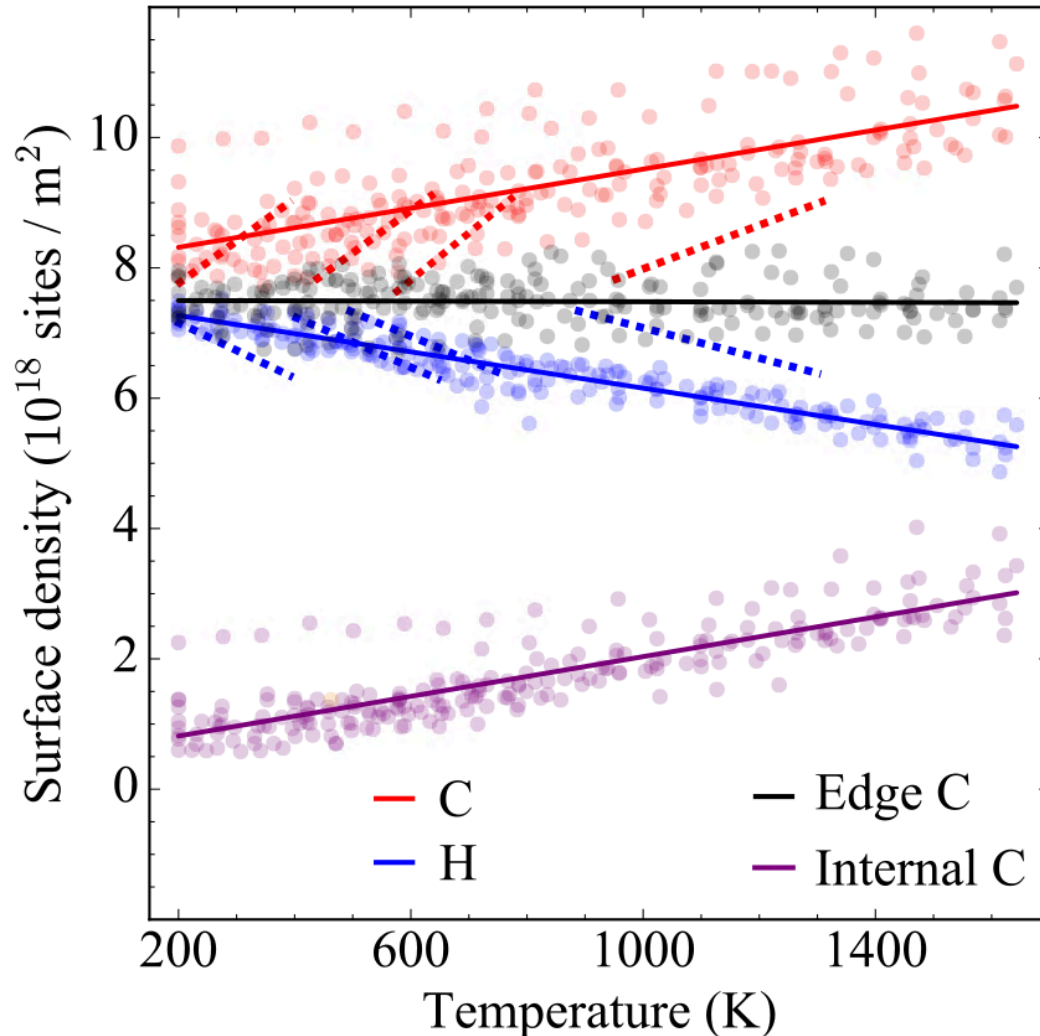


High temperature



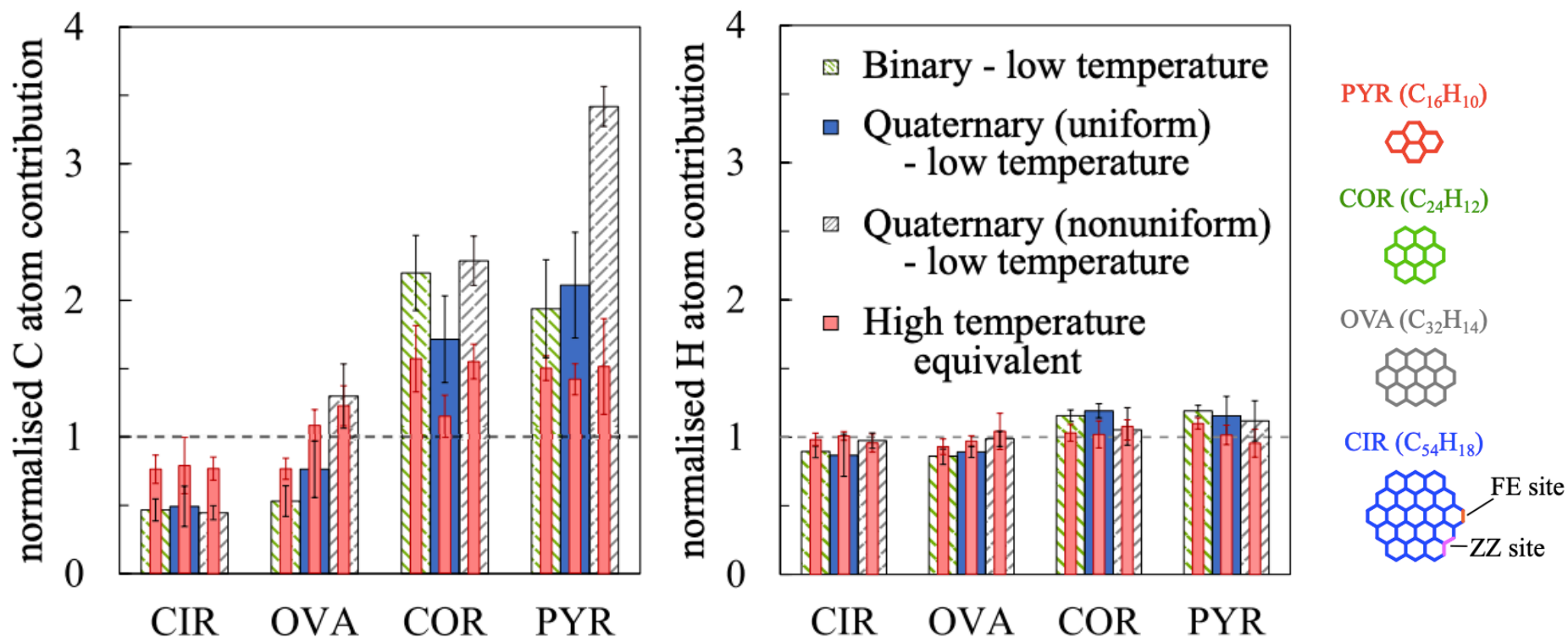
- Roughness increases with temperature
- Particle diameter and molecule sizes play a role in roughness
- Molecular composition (binary/quaternary) not very influential

Surface composition



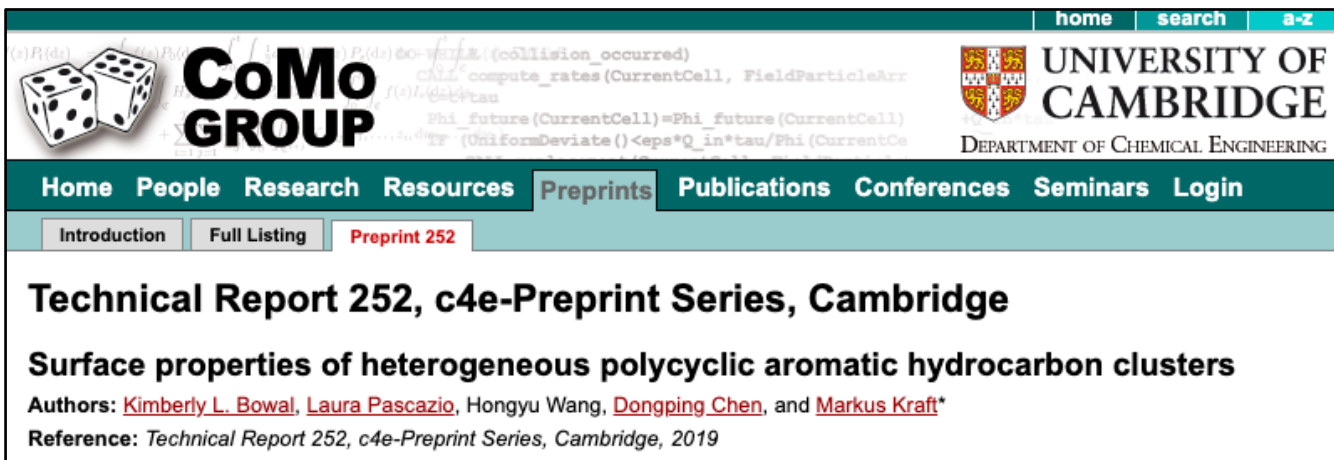
- H and C atoms: primarily dependent on temperature, explained by solid-like to liquid-like particle morphology
- EC does not change with temperature – can be described by molecule composition alone

Molecule type contributions



- Surface H atoms: All molecules contribute proportionately
- Surface C atoms: Large molecules contribute less than expected and small molecules contribute more – core-shell structure
- High temperatures move towards expected contributions

Summary



The screenshot shows the CoMo GROUP website header with navigation links: Home, People, Research, Resources, Preprints (selected), Publications, Conferences, Seminars, and Login. Below the header, there are tabs for Introduction, Full Listing, and Preprint 252 (selected). The main content area displays the title "Technical Report 252, c4e-Preprint Series, Cambridge" and the subtitle "Surface properties of heterogeneous polycyclic aromatic hydrocarbon clusters". The authors listed are Kimberly L. Bowal, Laura Pascazio, Hongyu Wang, Dongping Chen, and Markus Kraft*. The reference is "Technical Report 252, c4e-Preprint Series, Cambridge, 2019".

- Percentage of surface C and ZZ sites depend on particle size. H and FE sites are influenced by molecule size and ratio
- Particle roughness shows that surface area is significantly higher than spherical particle approximations
- Surface density values show us that surface densities of H, IC, and ZZ sites are dependent on temperature, while EC, FE site surface densities can be predicted from average molecule size
- Small molecules contribute more to cluster surface properties than large molecules

Thank you

