UNIVERSITY OF CAMBRIDGE

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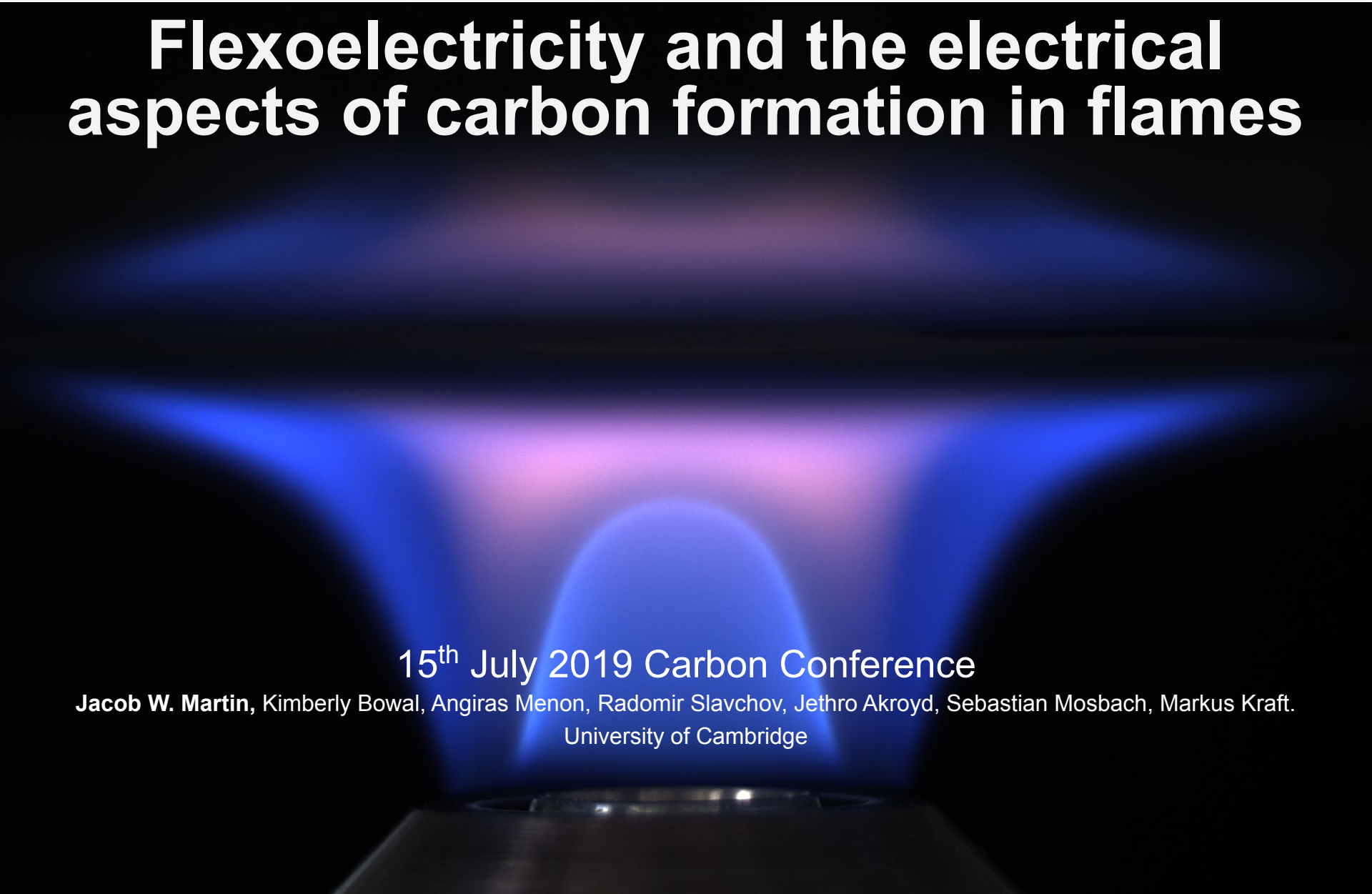
CAMBRIDGE CARES — CAMBRIDGE CENTRE FOR ADVANCED RESEARCH AND EDUCATION IN SINGAPORE LTD.

# Flexoelectricity and the electrical aspects of carbon formation in flames

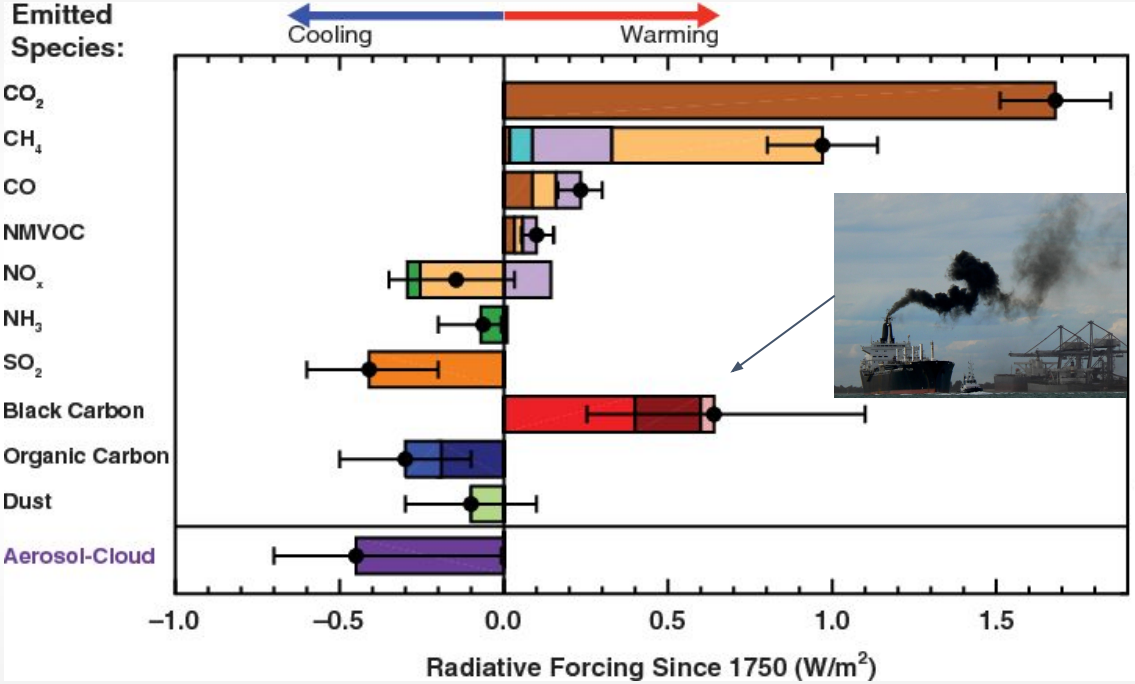


15th July 2019 Carbon Conference

**Jacob W. Martin,** Kimberly Bowal, Angiras Menon, Radomir Slavchov, Jethro Akroyd, Sebastian Mosbach, Markus Kraft.
University of Cambridge

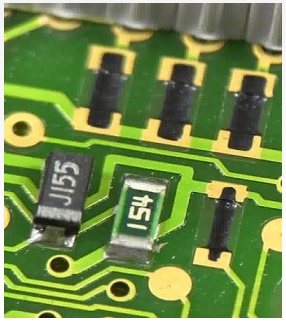
# Motivations

**POLLUTION - SOOT**



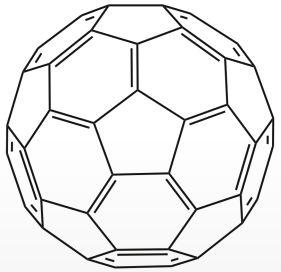

Fiore 2015

**PRODUCT - CARBON BLACK**



Conductive ink

Li-ion batteries

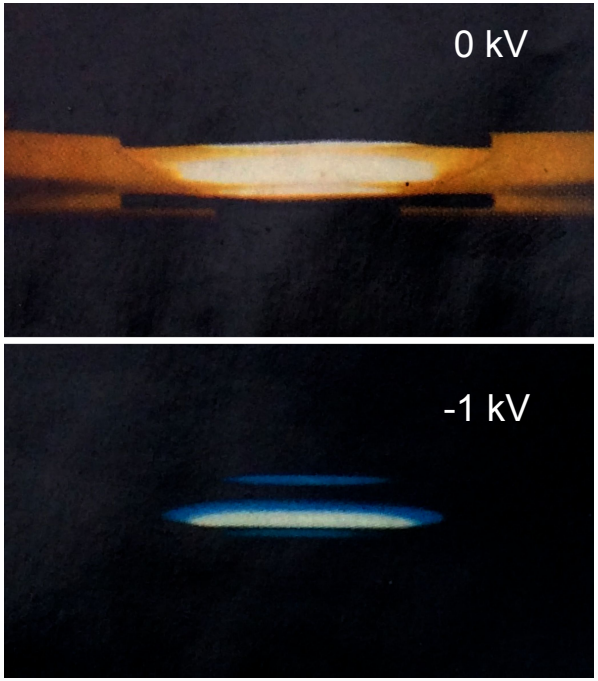


Fullerenes and nanotubes

HAOJIAN

# Electrical aspects of combustion

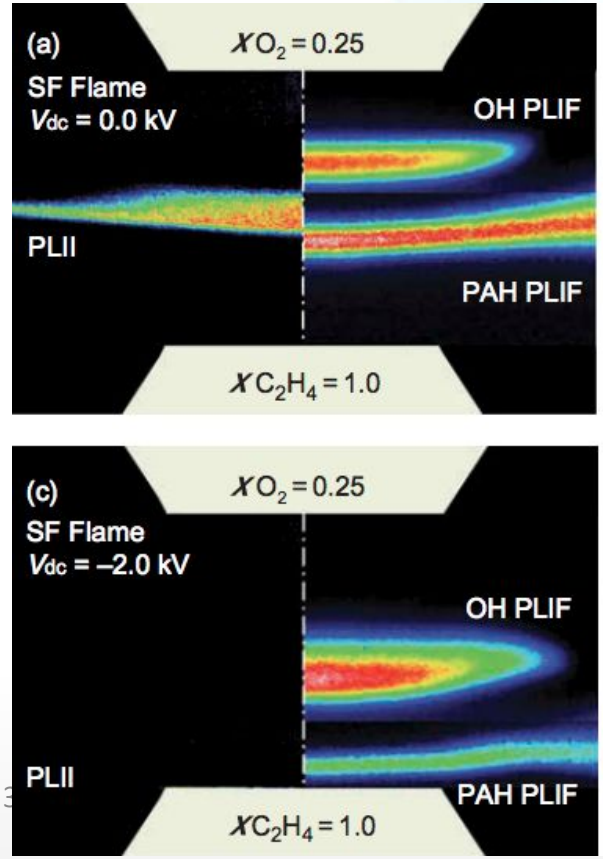
Brande 1814




Lawton and Weinberg 1959

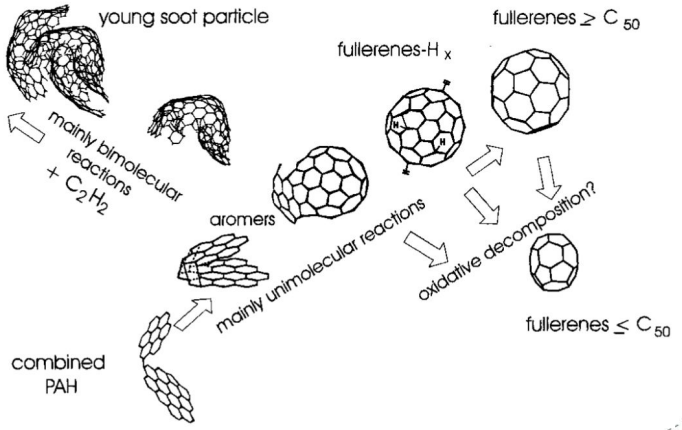
planar laser-induced incandescence

planar laser-induced fluorescence

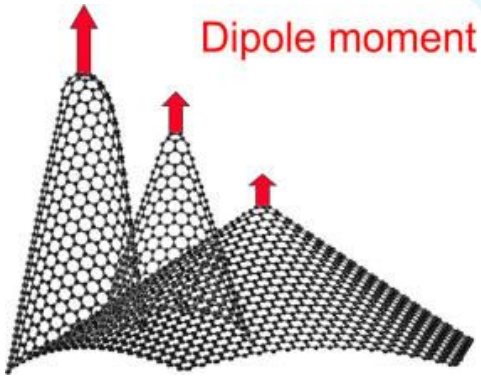



Park et al. 2014

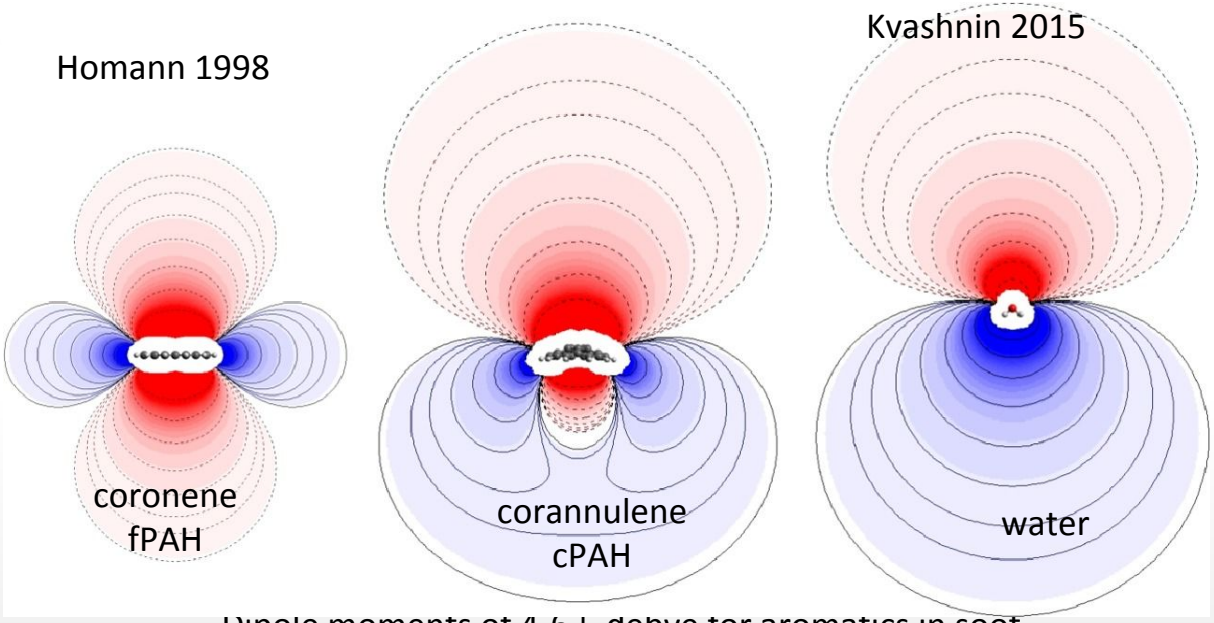
# Flexoelectricity and soot formation




Homann 1998



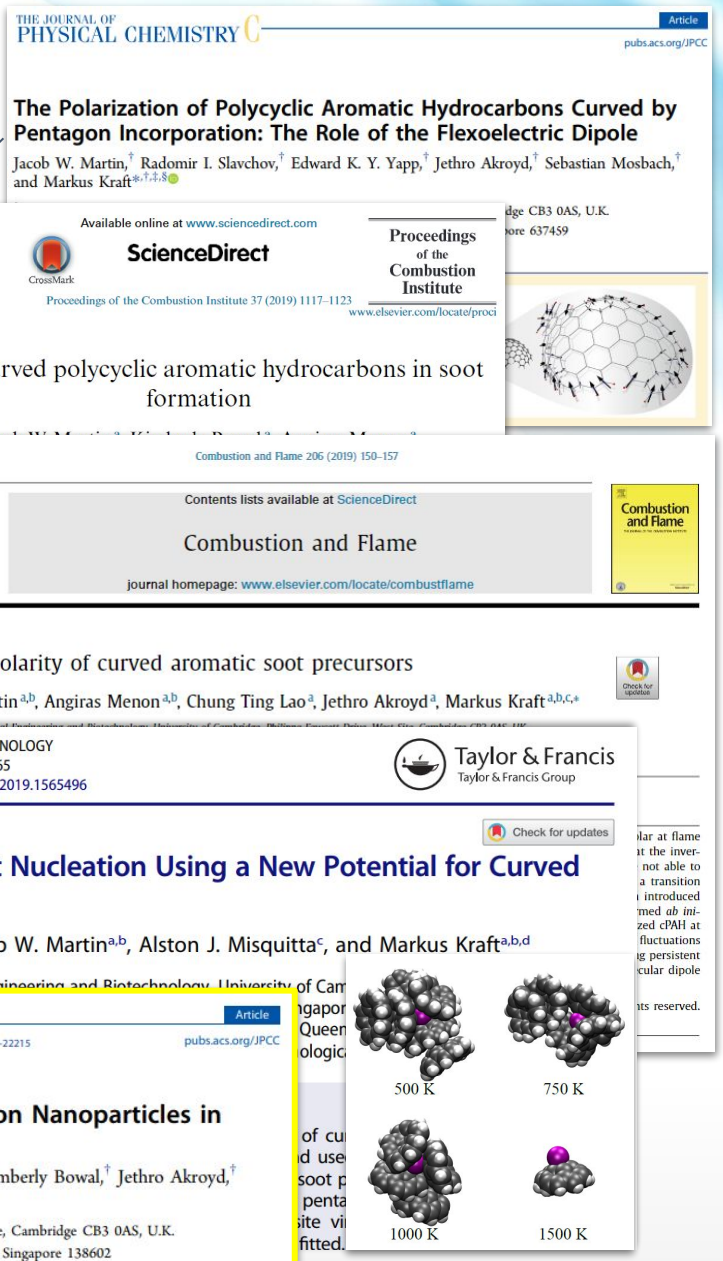

Kvashnin 2015




Dipole moments of 4-6.5 debye for aromatics in soot

# Questions to answer

- How do you describe the polarity of cPAH?
  - Flexoelectric constant
  - Developed multipole forcefields
- How well do they bind to each other?
  - Similar to flat PAH
- What is the minimum size to be polar?
  - 6 rings
- Are cPAH persistently polar in a flame?
  - Not above 10-13 rings
- Does polarity affect nucleation?
  - Yes no effect for fPAH
- **Are they present in soot?**

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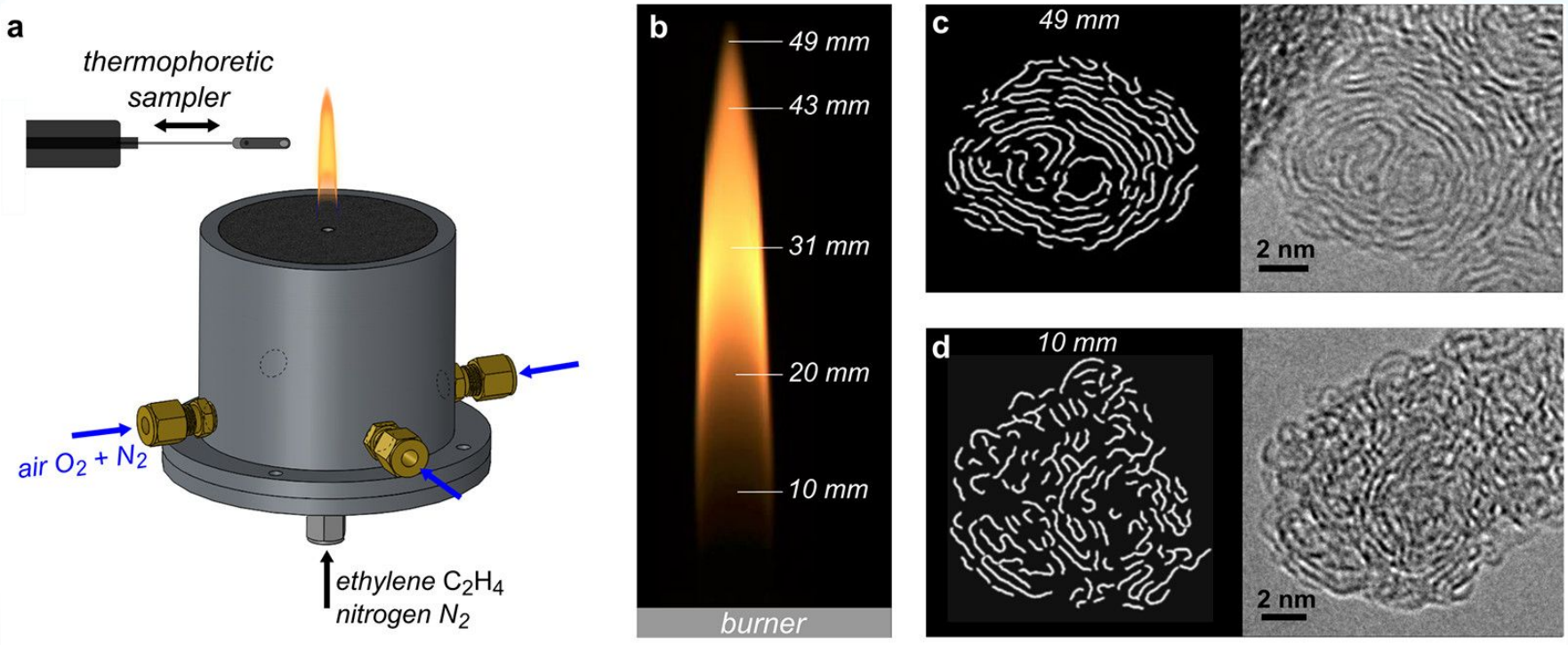
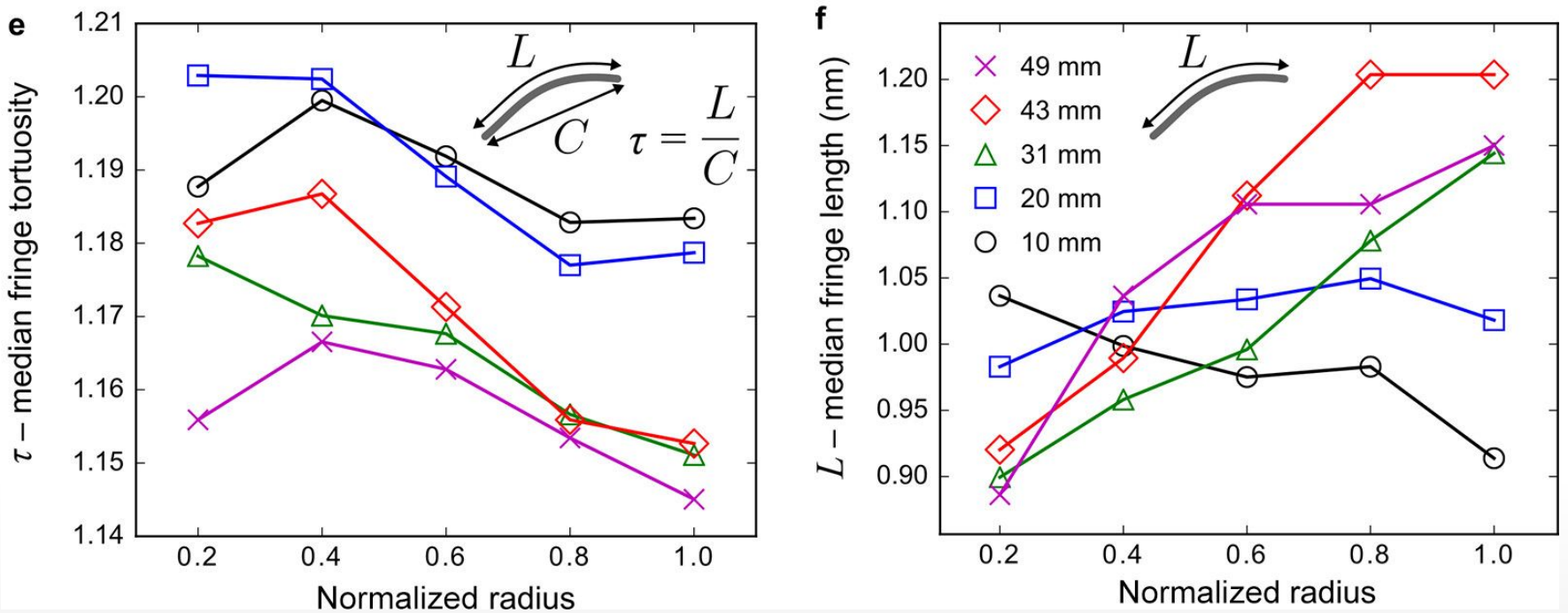
# Internal structure of soot particles




Martin, Jacob W., et al. "Flexoelectricity and the formation of carbon nanoparticles in flames." *The Journal of Physical Chemistry C* 122.38 (2018): 22210-22215.

# Quantifying curvature

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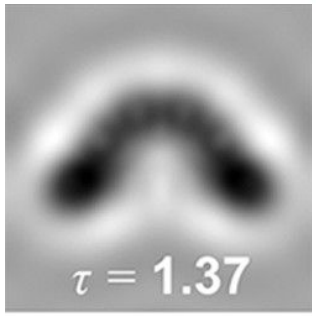
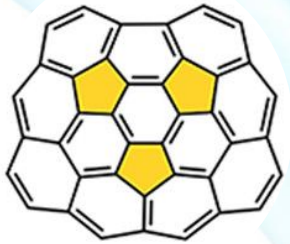
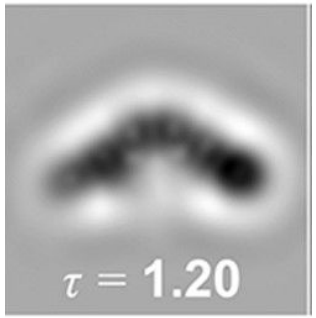
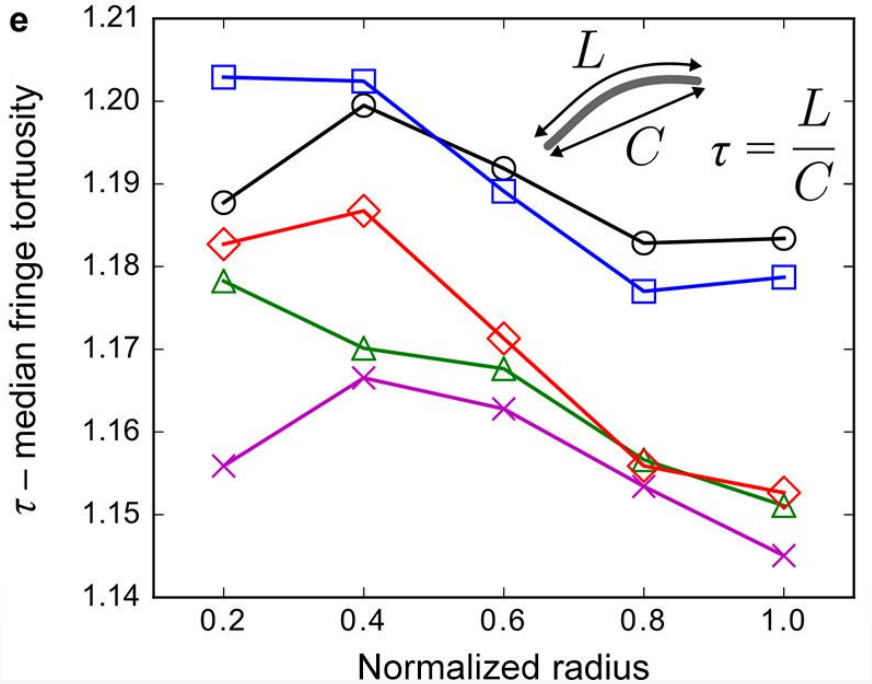
# Quantifying curvature

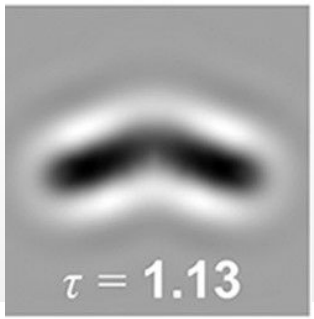





>60% of fringes at 10 mm HAB indicated
>1 internal pentagonal ring

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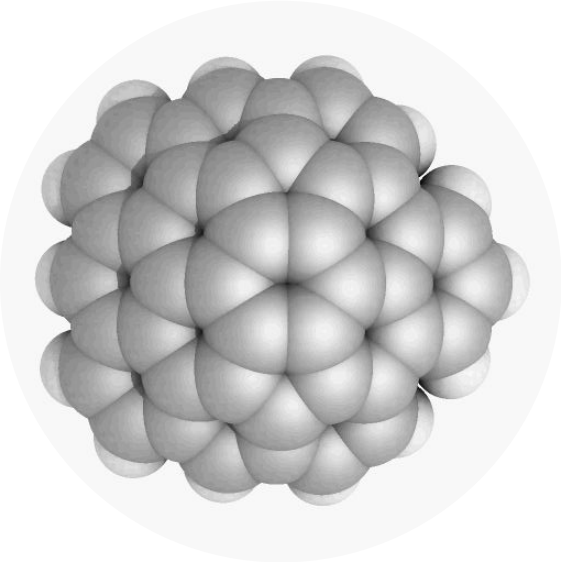
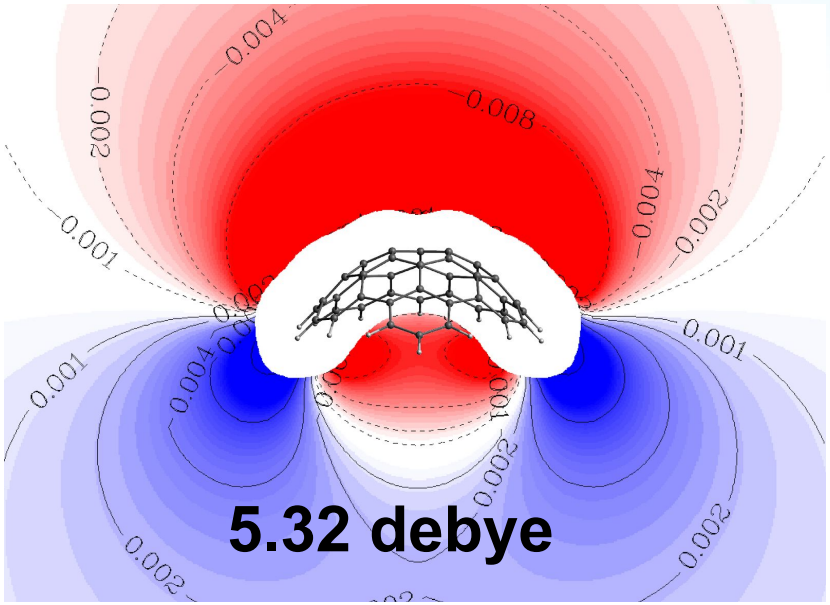
# Polarity



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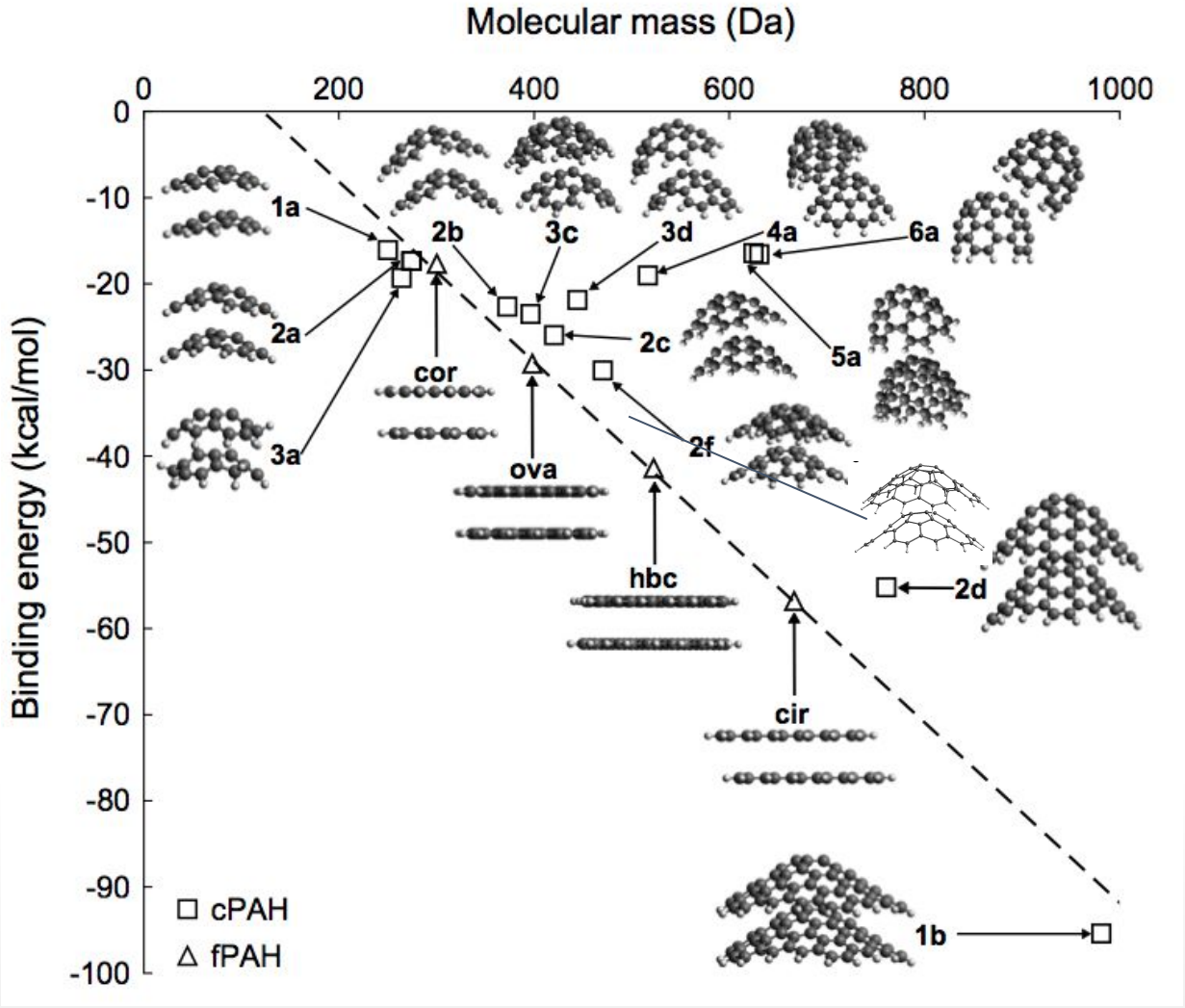
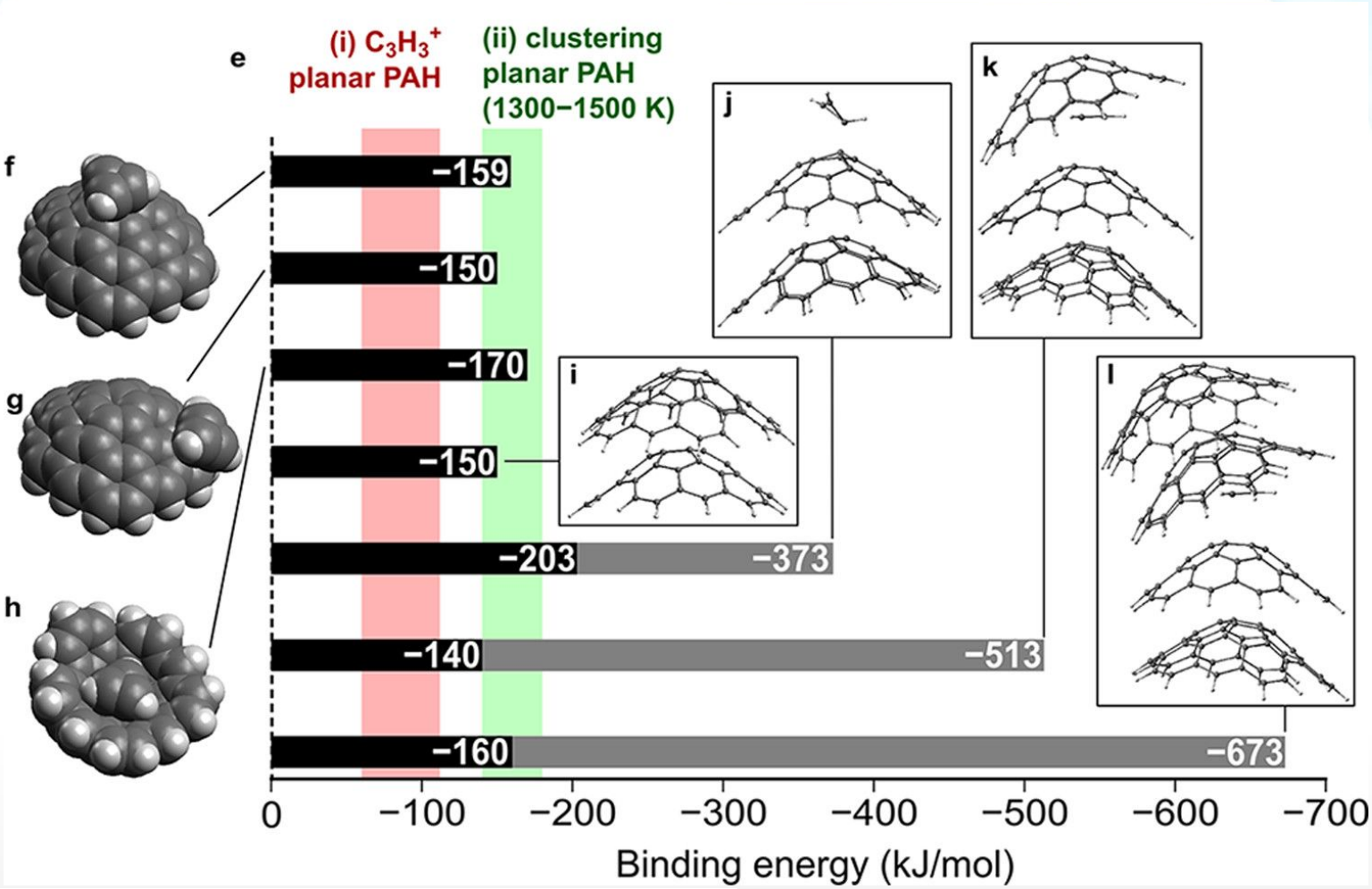
# Homogeneous nucleation



# Interaction with chemi-ons

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# Questions

- How do you describe the polarity of cPAH?
- How well do they bind to each other?
- What is the minimum size to be polar?
- Are cPAH persistently polar in a flame?
- Does polarity affect nucleation?
- **Are they present in soot?**
  - Yes - 1-2 pentagonal rings >60% of early soot
  - 4-6.5 debye (2 pentagon 15 rings 5.32 D)
  - a small number could cluster on cations

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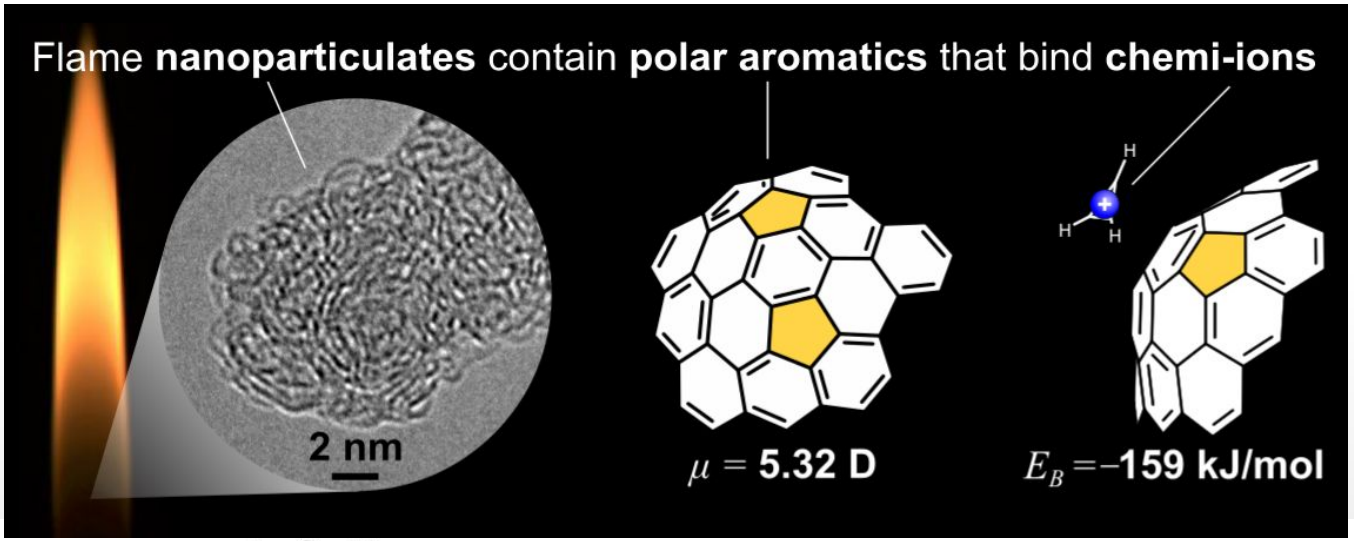
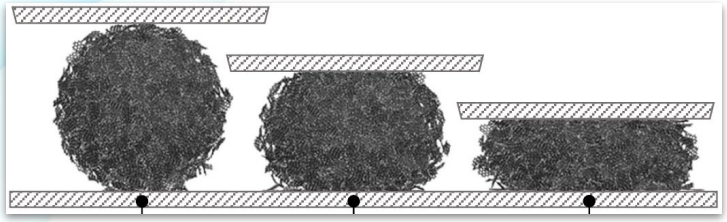
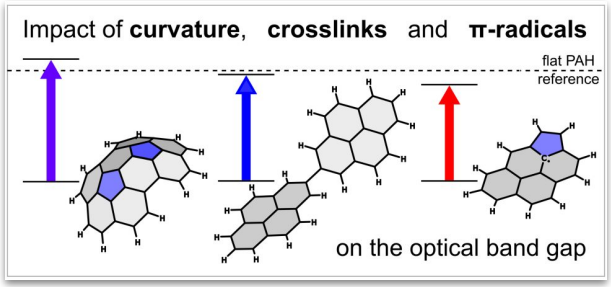


**WANT TO SEE MORE!**



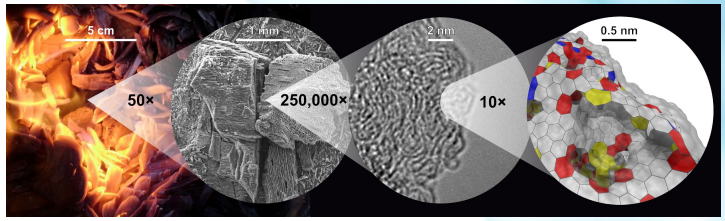
Degree of crosslinking in combustion carbons

**Pascazio Mon. 3:20 pm Rm 5**



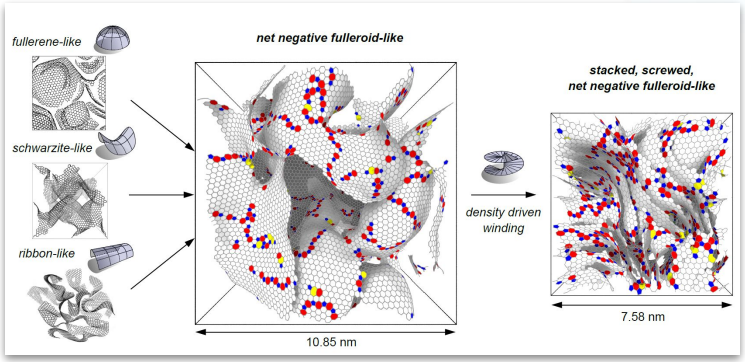

Impact of curved, crosslinks and radicals on the band gap of nanographenes

**Menon Thurs. 11:20 am Rm. 5**




Understanding the lack of fullerenes in fullerene-like carbons

**Martin Mon 3:40 pm Rm 2**




Topology of disordered carbons

**Martin Wed. 3:40 pm Rm. 5**

**Thanks for your attention**

**Thanks to the funder**

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This project is funded by the
**National Research Foundation (NRF)**,
Prime Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.

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