

# Flexoelectricity and the electrical aspects of carbon formation in flames

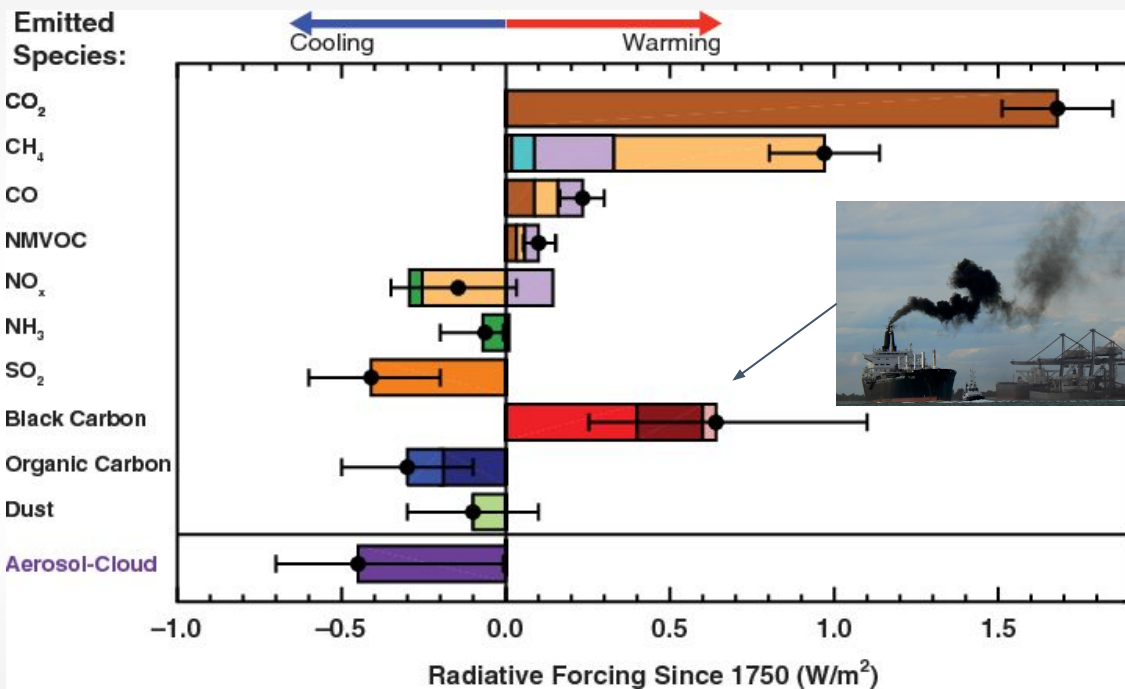
15<sup>th</sup> July 2019 Carbon Conference

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

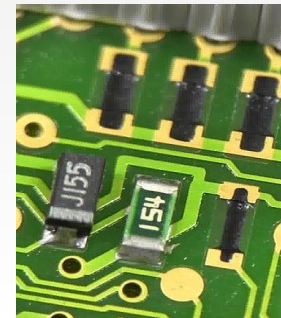
# Motivations

## POLLUTION - SOOT

## PRODUCT - CARBON BLACK



Fiore 2015



Conductive ink



Li-ion batteries



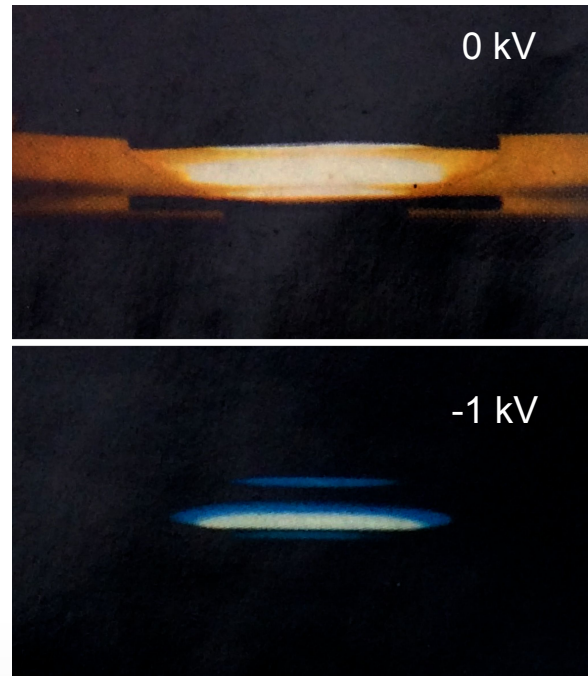
Fullerenes and nanotubes

HAOJIAN

# Electrical aspects of combustion

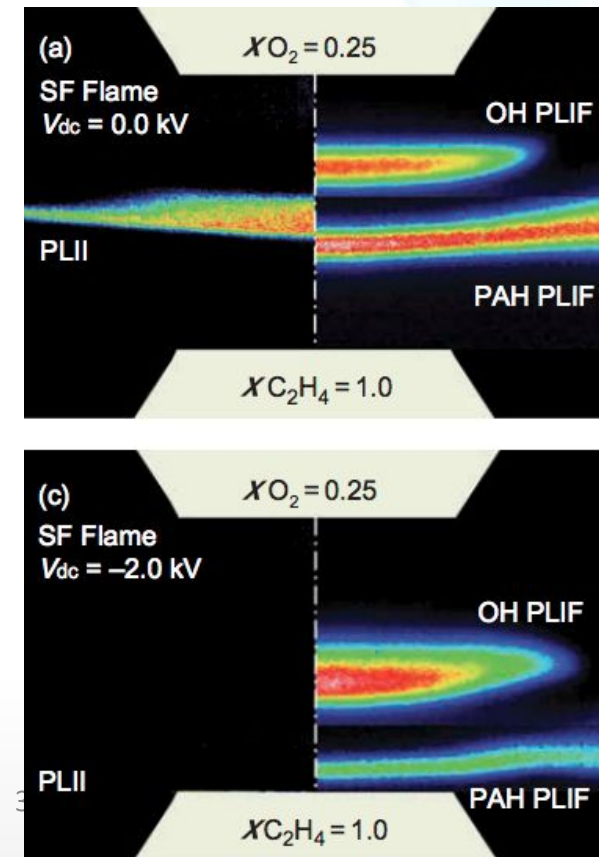


Brande 1814



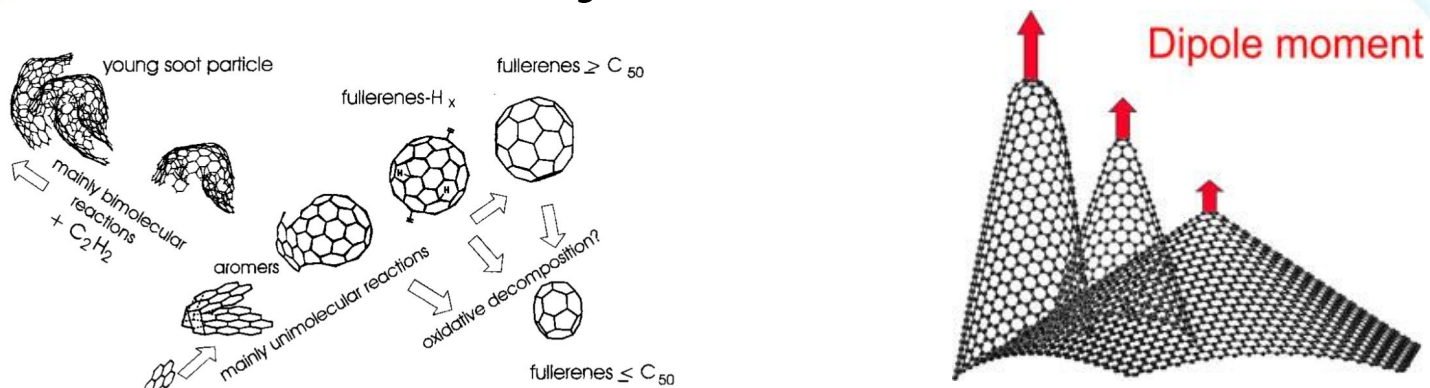
Lawton and Weinberg 1959

planar laser-induced incandescence      planar laser-induced fluorescence

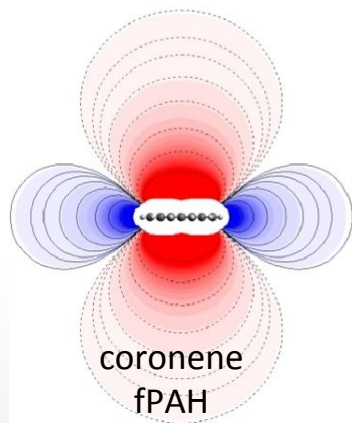


Park et al. 2014

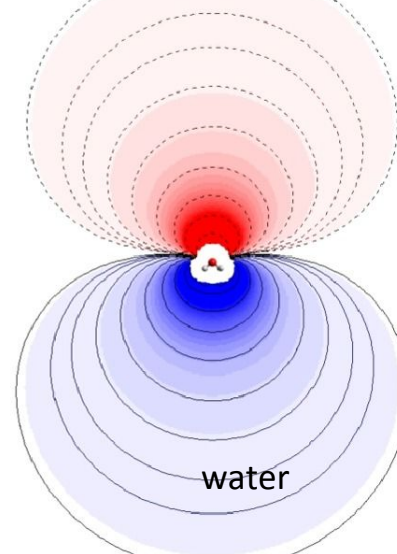
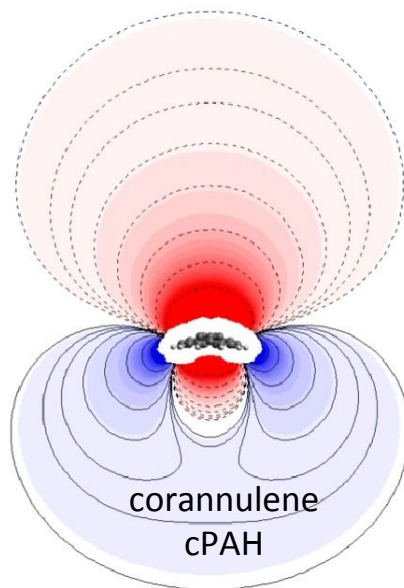
# Flexoelectricity and soot formation



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?

## The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole

Jacob W. Martin,<sup>†</sup> Radomir I. Slavchov,<sup>†</sup> Edward K. Y. Yapp,<sup>†</sup> Jethro Akroyd,<sup>†</sup> Sebastian Mosbach,<sup>†</sup> and Markus Kraft<sup>\*†,‡,§</sup>

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Proceedings of the Combustion Institute

Volume 37 (2019) 1117–1123

Article CB3 0AS, U.K. Article number 637459

**ELSEVIER**

Polar curved polycyclic aromatic hydrocarbons in soot formation

Combustion and Flame 206 (2019) 150–157

Contents lists available at ScienceDirect

**Combustion and Flame**

journal homepage: [www.elsevier.com/locate/combustflame](http://www.elsevier.com/locate/combustflame)



Dynamic polarity of curved aromatic soot precursors

Jacob W. Martin<sup>a,b</sup>, Angiris Menon<sup>a,b</sup>, Chung Ting Lao<sup>a</sup>, Jethro Akroyd<sup>a</sup>, Markus Kraft<sup>a,b,c,\*</sup>

**Check for updates**

COMBUSTION SCIENCE AND TECHNOLOGY  
2019, VOL. 191, NOS. 5–6, 747–765  
<https://doi.org/10.1080/00102202.2019.1565496>

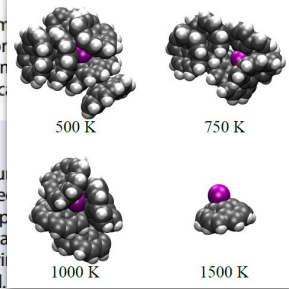
**Taylor & Francis**  
Taylor & Francis Group

**Check for updates**

## Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics

Kimberly Bowal<sup>a</sup>, Jacob W. Martin<sup>a,b</sup>, Alston J. Misquitta<sup>c</sup>, and Markus Kraft<sup>a,b,d</sup>

<sup>a</sup>Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge CB3 0AS, U.K.



## Flexoelectricity and the Formation of Carbon Nanoparticles in Flames

Jacob W. Martin,<sup>†,‡,§</sup> Maria Botero,<sup>‡,§</sup> Radomir I. Slavchov,<sup>†</sup> Kimberly Bowal,<sup>†</sup> Jethro Akroyd,<sup>†</sup> Sebastian Mosbach,<sup>†</sup> and Markus Kraft<sup>\*†,‡,§</sup>

<sup>†</sup>Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge CB3 0AS, U.K.

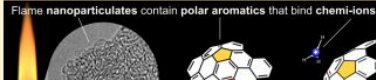
<sup>‡</sup>Cambridge Centre for Advanced Research and Education in Singapore (CARES), Singapore 138602

<sup>§</sup>Department of Mechanical Engineering, National University of Singapore, Singapore 117576

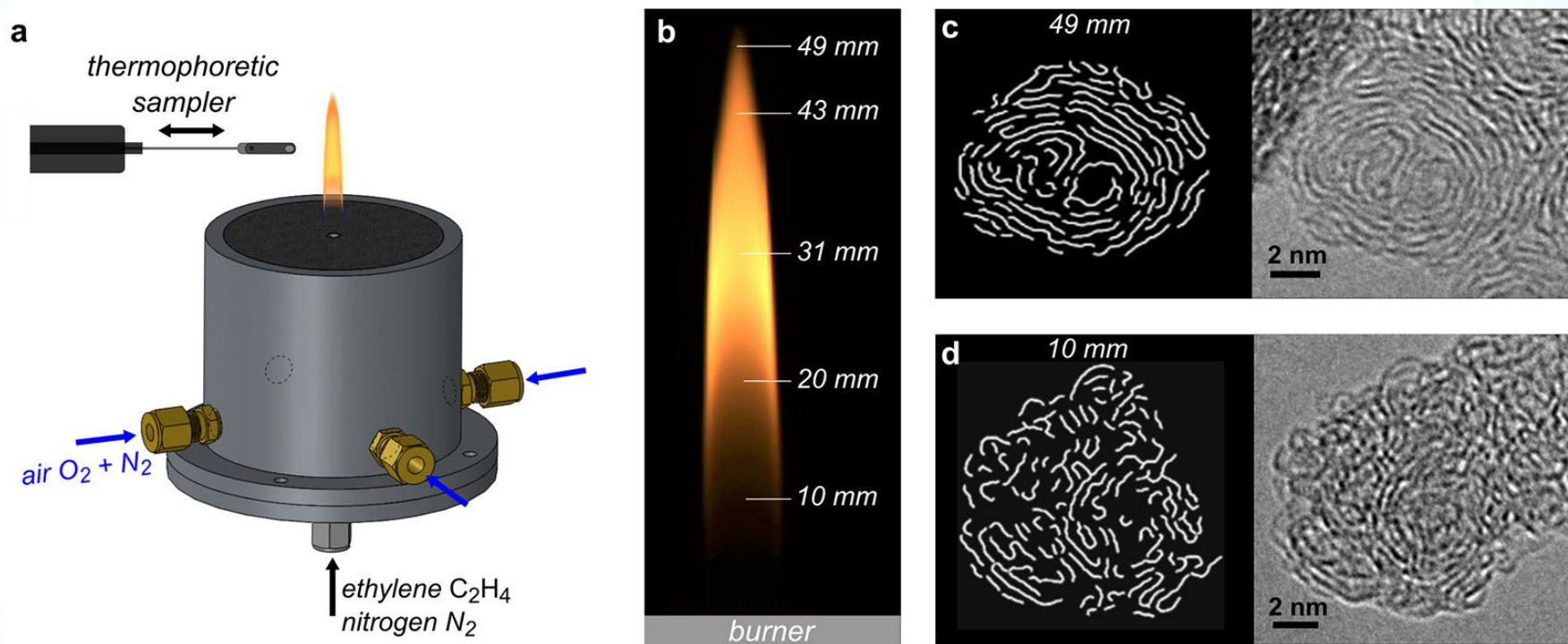
<sup>§</sup>School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore 637459

**Supporting Information**

**ABSTRACT:** The formation of carbon nanoparticles in flames involves a nucleation step that remains poorly understood. Experimentally, carbon nuclei formation is known to depend strongly on the electrical aspects of combustion, but modes of interaction between charged flame nanoparticles contain polar aromatics that bind chemi-ions

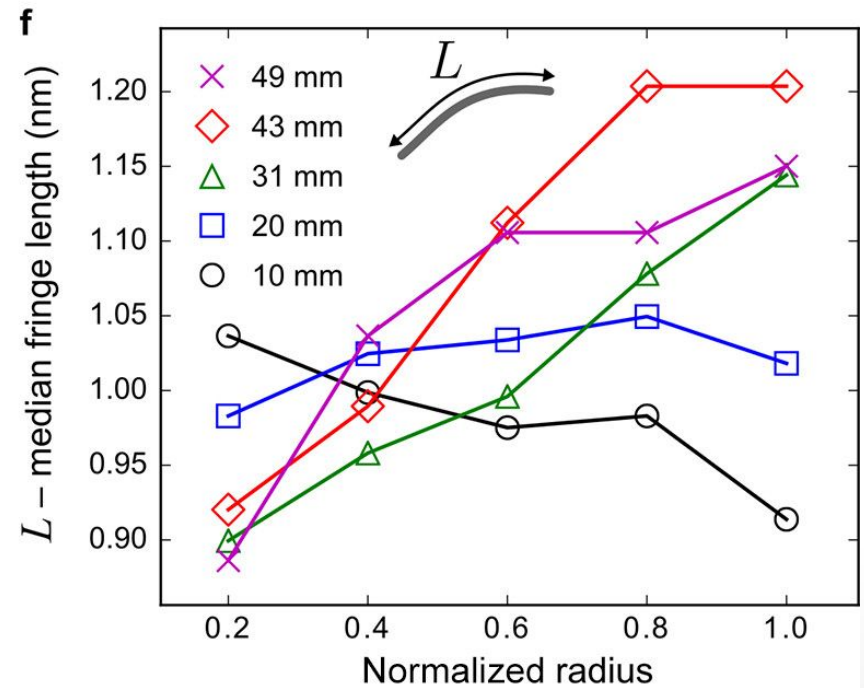
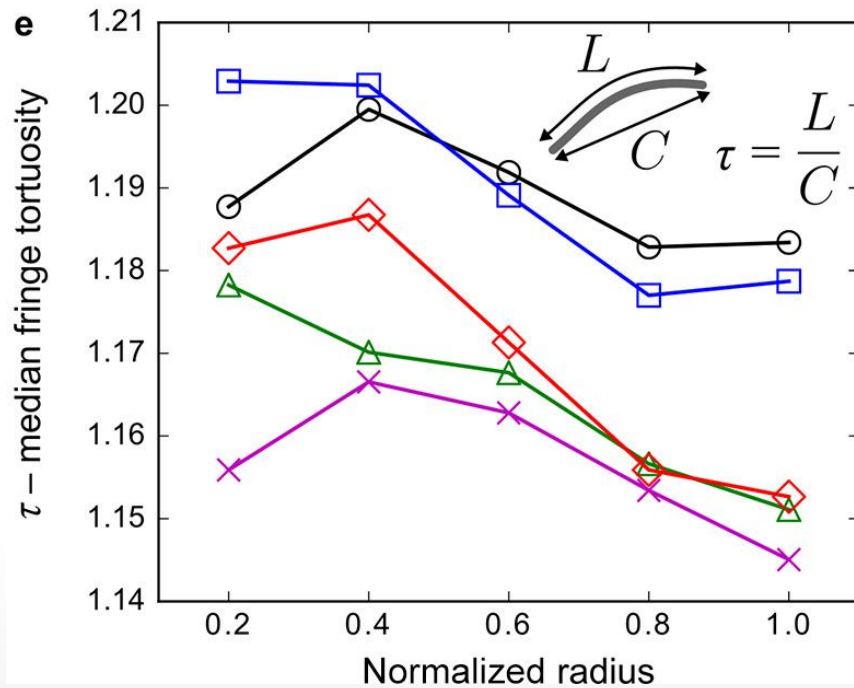


# Internal structure of soot particles



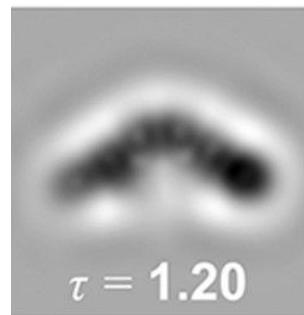
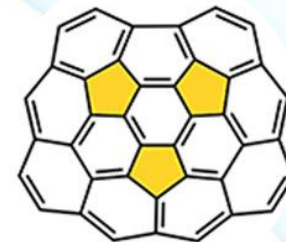
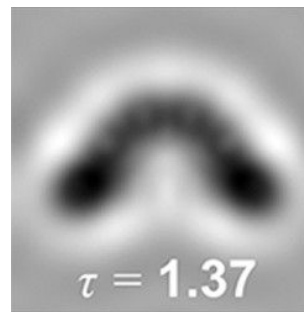
Martin, Jacob W., et al. "Flexoelectricity and the formation of carbon nanoparticles in flames." *The Journal of Physical Chemistry C* 122.38 (2018): 22210-22215.

# Quantifying curvature

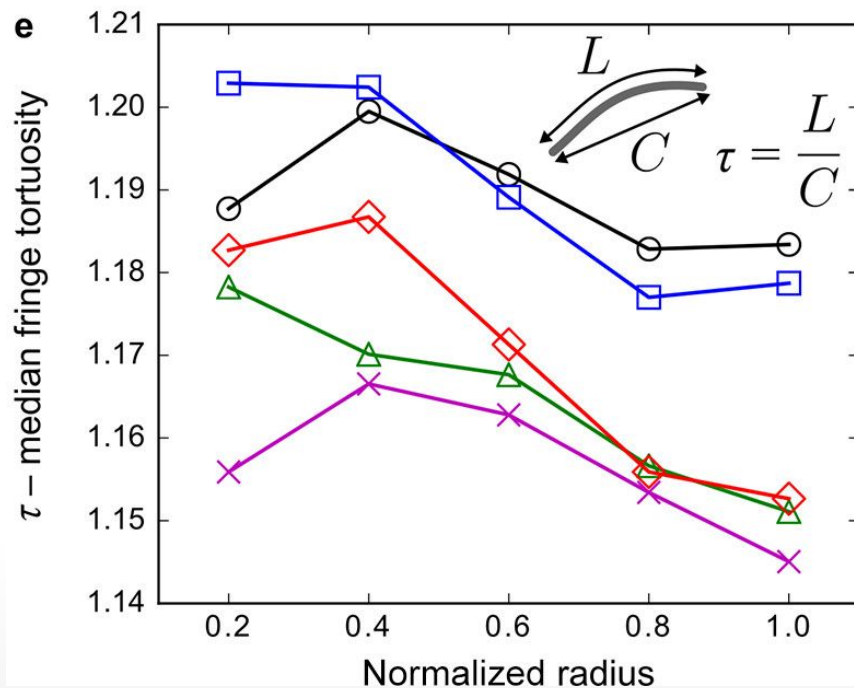
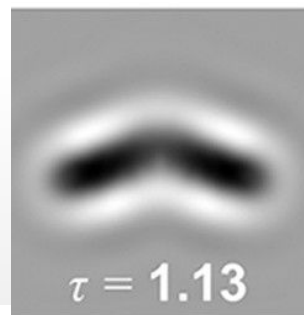


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# Quantifying curvature



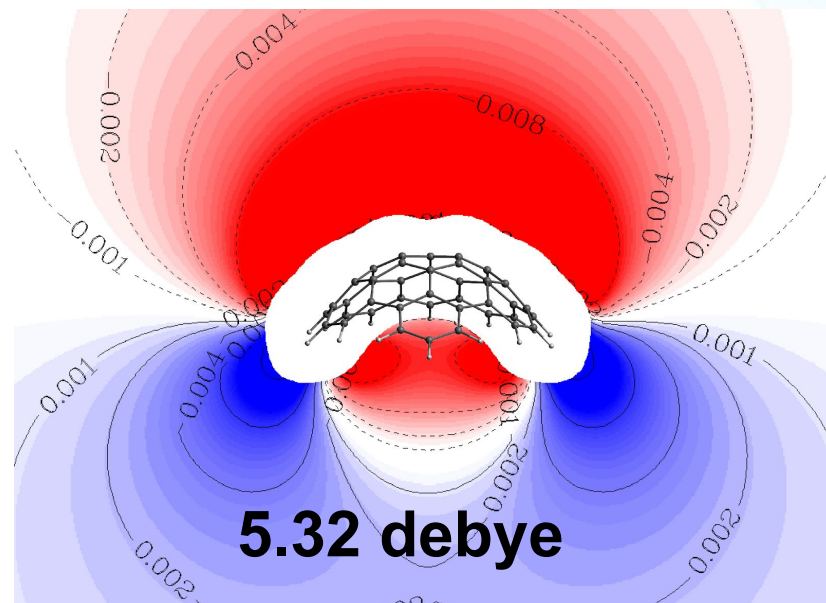
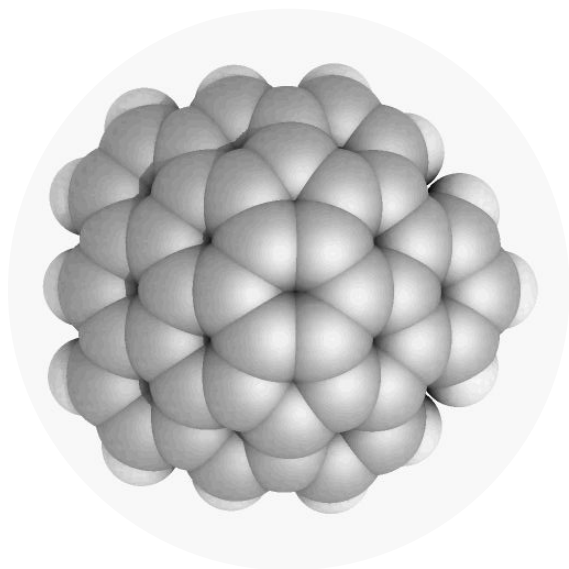
>60% of fringes at 10 mm HAB indicated  
>1 internal pentagonal ring



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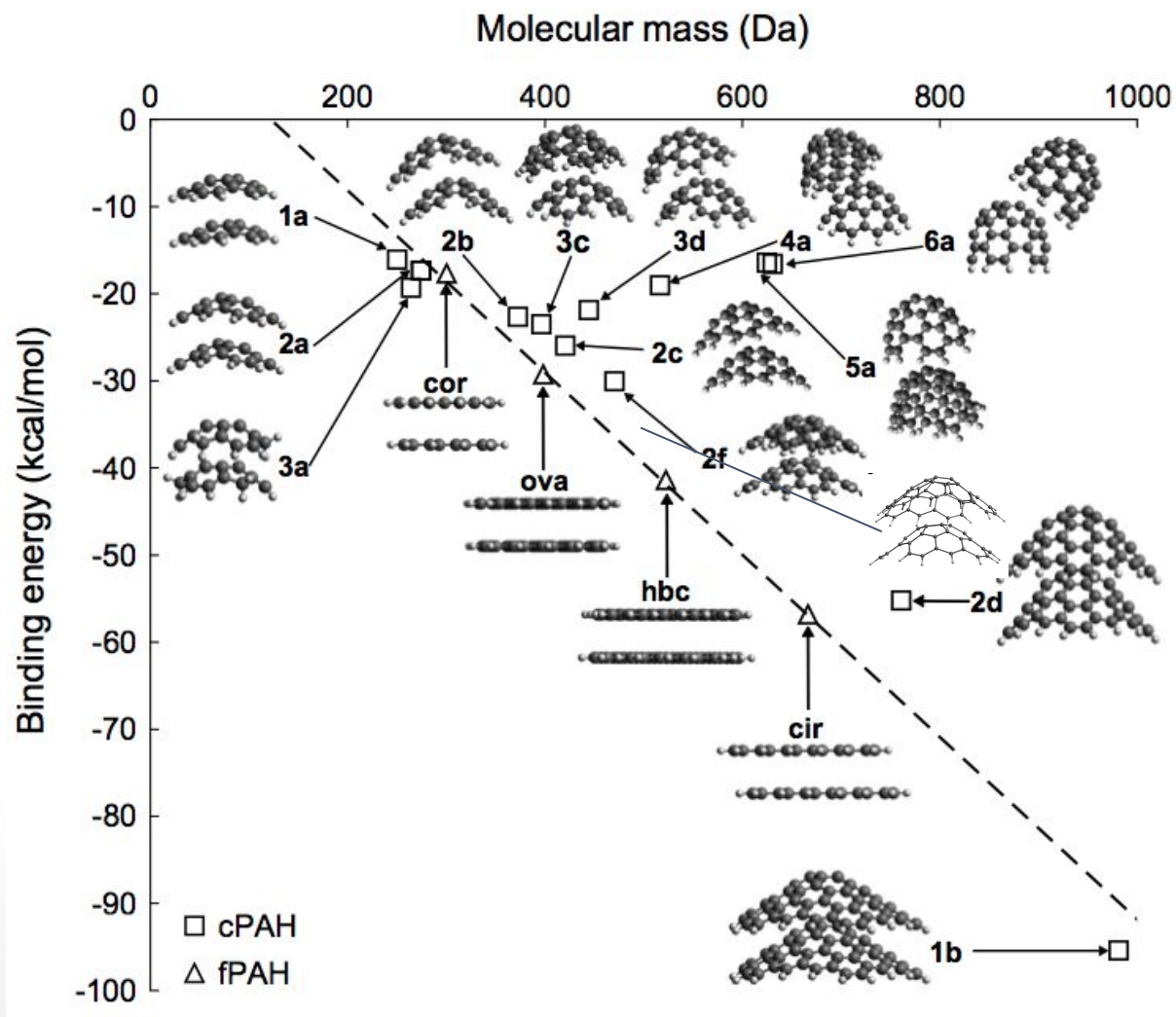


# Polarity

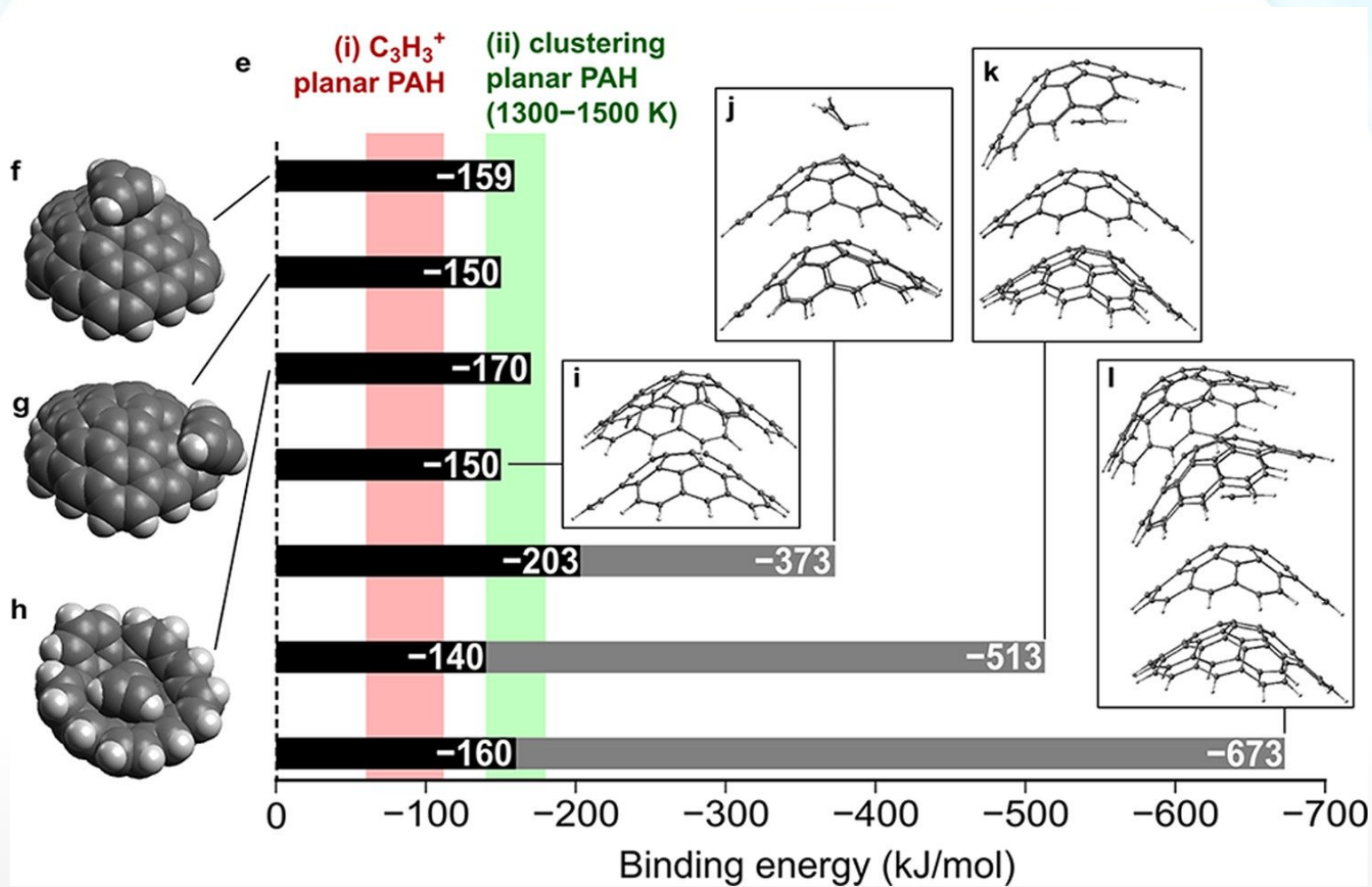


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# Homogeneous nucleation



# Interaction with chemi-ions

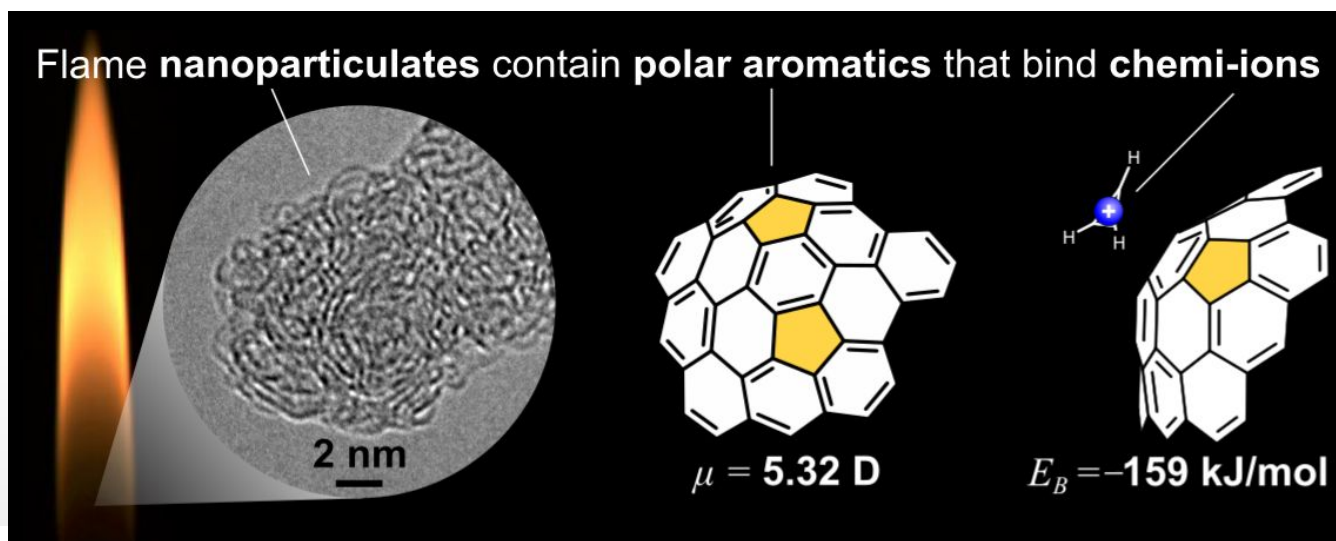


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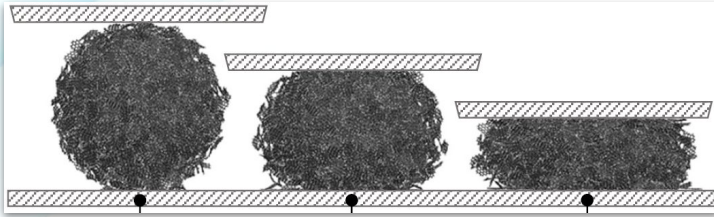
# Questions

- 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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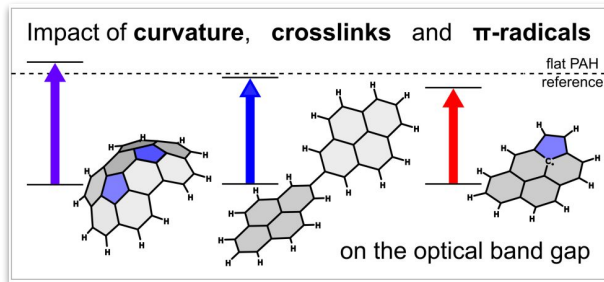


WANT TO SEE MORE!



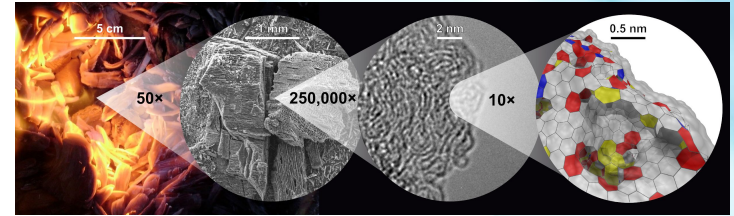
Degree of crosslinking in combustion carbons

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



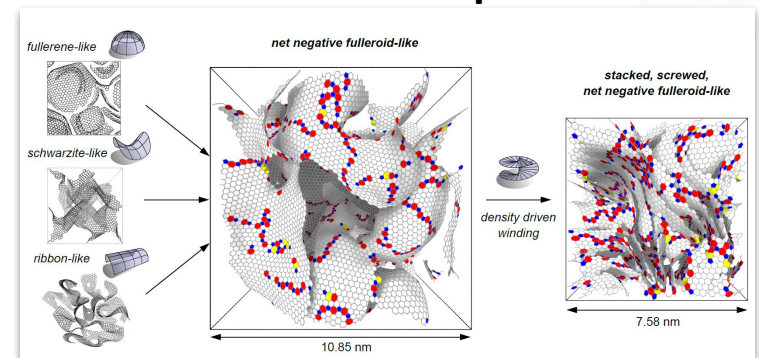
Impact of curved, crosslinks and radicals on the band gap of nanographenes

**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

**NATIONAL RESEARCH FOUNDATION**  
PRIME MINISTER'S OFFICE  
SINGAPORE

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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