Understanding the lack of fullerenes in fullerene-like carbons

15th Jul 2019 Carbon Conference

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Applications

**CARBON SEQUESTRATION - BIOCHAR**
- Why does biochar have such a long life?
- How do we optimise biochar for longevity?
- How does biochar break down?
- How does biochar interact with soil chemistry?
- How do heteroatoms become integrated?

**MATERIAL APPLICATIONS**
- Sodium-ion batteries (hard/soft carbon electrodes)
- Engineering pores for adsorbents
- Supercapacitors
- Hydrogen storage

Lehmann et al. 2006, Mitigation and Adaption Strategies for Global Change 11, 403-427


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Fullerene-like or non-graphitising

Microcrystalline model
Biscoe and Warren 1942

Crosslinked microcrystallite model
Franklin 1951

Ribbon model
Jenkins and Kawamura 1971

Where are the $C_{60}$?
Should we expect to see $C_{60}$?

C$_{60}$ discovered
Kroto et al. 1985

Schwarzite proposed
Mackay and Terrones 1991

Fullerene-like model
Harris and Tsang 1997

Ribbon-like

No $C_{60}$ in many charcoals
Bourke et al. 2007

No $C_{60}$ in glassy carbon
Sedo et al. 2006

Graphene triad ribbon model
McDonald-Wharrey et al. 2015

$C_{60}$ extracted from soot
Heymann et al. 1994

Fullerene-like model
Harris and Tsang 1997

Line dislocation imaged
Guo et al 2012

Ribbon structures
Guo et al. 2012
Where is C\textsubscript{60} in fullerene-like carbons?

PREPARING SOOT- AND TAR-FREE CHARCOAL

Microlab downdraft gasifier from Fluidyne

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Jacob W. Martin
Where is \( \text{C}_{60} \) in fullerene-like carbons?
Appears fullerene-like

HRTEM and RAMAN SPECTROSCOPY

HRTEM 200 kV
Should we expect to see $C_{60}$ fullerene?
Should we expect to see $C_{60}$ fullerene?

C_{60}/C_{70} consumed through coalescence

Giant fullerene formation

Oxygenated fragments

heated arc-carbon

Non-graphitising carbon
wood charcoal
Nanostructure of Gasification Charcoal (Biochar)

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ABSTRACT: In this work, we investigate the molecular composition and nanostructure of gasification charcoal (biochar) by comparing it with heat-treated fullerene soot. Using ultrahigh resolution Fourier transform ion-cyclotron resonance and laser desorption ionization time-of-flight mass spectrometry, Raman spectroscopy, and high resolution transmission electron microscopy we analyzed charcoal of low tar content obtained from gasification. Mass spectrometry revealed no magic number fullerenes such as C_{60} or C_{70} in the charcoal. The positive molecular ion m/z 701, previously considered a graphitic part of the nanostructure, was found to be a breakdown product of pyrolysis and not part of the nanostructure. A higher mass distribution of ions similar to that found in thermally treated fullerene soot indicates that they share a nanostructure. Recent insights into the formation of all carbon fullerenes reveal that conditions in charcoal formation are not optimal for the formation of fullerenes, but instead, curved carbon structures coalesce into fulleroid-like structures. Microscopy and spectroscopy support such a stacked, fulleroid-like nanostructure, which was explored using reactive molecular dynamics simulations.
Implications for reactivity

Implications for adsorption

Flexoelectricity

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

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

Menon Thurs. 11:20 am Rm 5

Investigating the self-assembly and structure of nanoparticles containing curved carbons

Bowal Tues. 4:20 pm Rm 2

Thanks to all collaborators
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Thanks for your attention
Microlab gasifier

Experimental downdraft gasifier was developed with Mr. Doug Williams from Fluidyne gasification

Wood block fuel consumption 4.5 kg/hr
Maximum output 9.8 Nm3/hr
Test duration 20 mins
Hopper volume 3 L
Blast tube, cyclone, cooling and sawdust filter

Currently installed at the University of Ulster.