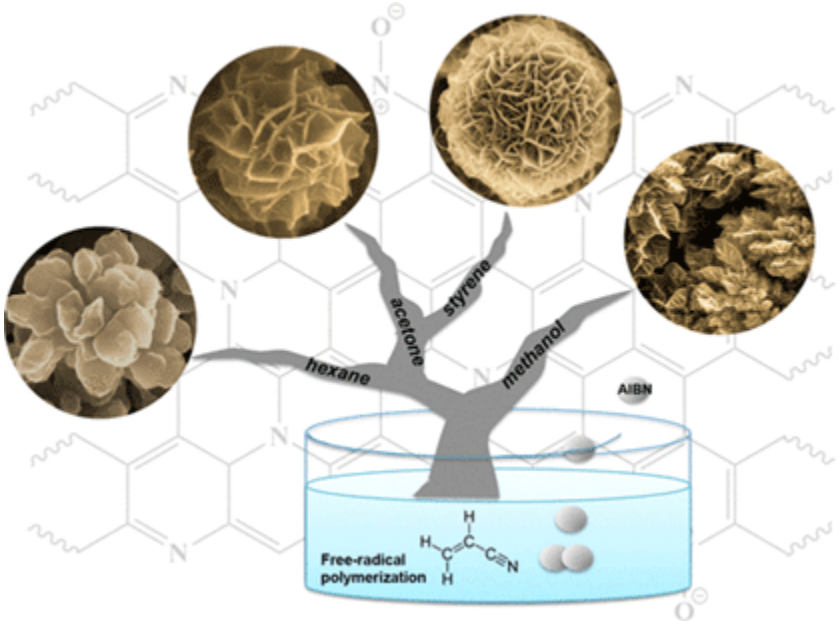
Docket #: S18-114

Simple synthesis of uniform carbon flower superstructures for electrocatalysts and other energy and environment applications

Engineers in Professor Zhenan Bao's laboratory have developed a simple, low-cost, tunable, one-step polymerization process followed by pyrolysis for producing uniform carbon particles with a variety of different superstructures (flower, petals, pompom shapes around 1um). Three-dimensional hierarchical porous carbon materials with flower-like superstructures provide highly accessible surface area and facilitate ion transport for high-rate capability which is valuable for energy applications. However, traditional synthesis of these geometries has been difficult and produced low quality materials that do not have regular, predictable structures. This new tunable process solves that problem using a one-pot, free-radical polymerization and self-assembly process that controls structure and porosity through solvents and co-monomers. The resulting carbon particles have uniform structure and desirable electrical properties. This method opens the possibility to synthesize carbon materials in a simple and controlled way with unique morphology, high surface area and tunable heteroatom content for future applications in electrochemical energy conversion and storage, such as supercapacitors, electrocatalysts and lithium-sulfur batteries, waste water treatment and gas storage.



Synthesis of carbon flower superstructures: *This schematic image shows the variety of structures formed by varying the solvents for this simple polymerization process. Additional shapes and pores can be introduced by incorporating other co-monomers.*

Stage of Research

The inventors have synthesized 50 g of uniform polyacrylonitrile materials that were readily converted to carbon particles with tunable porosity via gas treatment methods (this can be easily scaled up for industrial purpose). The resulting carbons had diameters around 750 nm, exhibited high N-doping concentration (7-15 at%) and good performance as electrocatalysts. In addition, the inventors were able to accurately determine solvents for preparing particles with desired shapes by using Hansen solubility parameters.

Applications

- **Versatile carbon black/carbon materials** with end-user applications such as:
  - Energy - electrocatalysts (such as oxygen reduction reaction to produce H_2O_2); supercapacitors
  - Batteries/electrochemical - lithium sulfur and other batteries; thermo-switching polymer composite for safer batteries

    - Environment - water treatment/purification; gas adsorption and storage
    - Other - pressure sensors (fillers for conductive composites), rubber mechanical strength enhancement

Advantages

- **Easy synthesis** - simple, one-step polymerization and self-assembly process, followed by pyrolysis, to produce small particles with a variety of carbon superstructures
- **Low cost materials** - the precursors are cheap and carbon is an inexpensive, earth abundant element
- **Uniform particles with tunable properties:**
    - shapes of polymer structure can be tuned by changing synthetic conditions (e.g., using different solvents or incorporating other co-monomers)
    - can produce flower, pompom, hairy leaf and petal shapes around 1 um
    - porosity can be adjusted to optimize desired end-user application
- **Advantages of flower superstructure** - unique hierarchical porous carbon shapes with interconnected pores:
    - provide highly accessible surface area
    - offer open structure with more exposed active sites
    - extended nanopetals intersecting each other to facilitate transport of ions and electrons for good electrical properties:
        - conductivity ~0.5 S/cm
        - high rate capability from fast ion transport
    - offer high N loading

Publications

- Chen, S., Koshy, D. M., Tsao, Y., Pfattner, R., Yan, X., Feng, D., & Bao, Z. , "Highly Tunable and Facile Synthesis of Uniform Carbon Flower Particles," *Journal of the American Chemical Society* (2018), 140(32), 10297-10304. doi:10.1021/jacs.8b05825

Patents

- Published Application: 20210284537
- Issued: 11,702,339 (USA)

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