



Center for Renewable Carbon: Renewable Carbon for Energy Storage Systems

Producing natural and synthetic graphite is extractive and fossil-fuel based. A critical need exists for alternative graphite feedstocks that are less environmentally burdensome and free of supply constraints. As of today, no domestic supplies of graphitic carbon exist in the U.S. except for synthetic graphite. A cheap, domestic graphite supply is essential and urgent as each new electric vehicle will need 67 kg of graphite on average.

Drs. David Keffer and David Harper developed nanocrystalline carbon composites from lignin, demonstrating novel ion capture mechanisms for energy storage. Techno-economic analysis of converting lignin to carbon materials proves that it is not only feasible but chemicals and fuels are also made in the process. To further enhance this work's value, we recently demonstrated that cellulose pulp, co-produced with lignin, can be used as the primary component in composite materials to replace automobile plastics in pursuit of the fully recyclable vehicle in collaboration with Volkswagen.

Starting from total x-ray and neutron scattering data, we developed a physics-based model to

capture the structure of lignin-derived nanocrystallite carbon composites as a function of processing temperature and feedstock. From these atomistic models of the carbon structure, we visualized the development and distribution of graphitic domains in an amorphous matrix. We use this tool to evaluate the binding of Li ions in carbon materials using classical molecular dynamics simulations (MD) for energy storage (battery) applications.

We developed a blueprint for determining the processing-structure-property-performance (PSP) relationships in transforming lignin feedstocks into nano-graphitic composites and other nanomaterials, such as ultra-high surface area (> 3,200 m²/g) activated carbons for supercapacitor electrodes. The integrated experimental and computational work to date provides detailed analytical models that can be used for various carbon applications. In the process, we have

generated software that can be used by any scientist wanting to build models spanning from the atomic scale to the mesoscale based on total x-ray or neutron scattering data of composites with amorphous and crystalline domains.

Graphitic carbon materials are used in many commercial applications, such as battery anodes, refractory resins, filtration, and many others. Lignin is a byproduct of paper manufacturing or biofuel production that is burned for process energy or discarded as waste. undervalued co-product into high-value graphitic carbon materials. Not only does this address a supply issue for battery manufacture, it provides a much-needed high-value product to help rejuvenate a once-thriving pulp industry in rural areas. Techno-economic analysis proves that converting lignin to carbon materials is feasible, and chemicals and fuels are also made along the way. potential to reduce GHG emissions by 52–86% compared to natural graphite and by 95–97%.

