

Quantifying the Effects of Carbon Sub-nanoporous Structures on Electrochemical Capacitance

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In an electrochemical double layer capacitor (EDLC), intrinsic capacitance of the surface available for charge storage is depicted by the equation below [1]:

$$C = \epsilon_r \epsilon_0 A/d;$$

where C = Capacitance, ϵ_r = permittivity of the electrolyte, ϵ_0 = permittivity of a vacuum, A = area available to store charge, d = distance separating charge.

When increasing the surface area of a porous activated carbon, researchers have created EDLC's with materials containing micropores (0-2 nm) [2-4]. The more recent of the latter citations, reported these microporous materials to have lower capacitance as the predominant pore width approached 1 nm [2]. Contrarily, when pores were tailored to approximately the width of electrolyte ions found in the supercapacitor electrolyte, the capacitance exceeded the values found in meso- or macro-porous materials [2]. In support of the increase in capacitance, molecular modeling has linked the presence of micropores to capacitance [5, 6]; however, the process to quantify capacitance of a supercapacitor cell to micropore structure is still not well understood [7, 8].

Interestingly, Kaus shows that the time that electric charge is held within a supercapacitor affects the extent to which the cell will develop a potential after a discharge cycle or lose potential after a charging cycle [7]. This particular effect has been attributed to the redistribution of ions confined within micropores as a result of limited ion mobility. Building an analogy on the idea of limited ion mobility in nano-confined spaces, this study is used to determine if the contribution of various pore sizes to the electrochemical capacitance can be distinguished using variations in the charging time. As an example, we aim to create a situation where the capacitance measured for materials with solely mesopores or micropores can be compared as a function of charge redistribution.

In order to quantify of the distribution of micropores within carbon materials used in this study, physisorption isotherms were collected using nitrogen and carbon dioxide as the adsorbate. For nitrogen based data we used a quenched solid density functional theory kernel to model a combination of slit and cylindrical pores greater than 1 nm in size [9]. For carbon dioxide based data, anon-local density functional theory kernel for slit-shaped pores was used to characterize pores less than 1 nm in diameter [10]. The surface analysis data is presented in **Table 1**.

The activated carbon materials are then made into an electrode film containing 90wt% activated carbon, 6% carbon black and 4wt% PTFE. To create a supercapacitor cell, two electrodes are separated by a porous polysulphone membrane and are placed between two nickel wire mesh current collectors. The cell is then sandwiched between two acrylic plates and then secured with stainless steel screws.

The capacitance and charge redistribution for these materials will be measured.

		Peak Center nm	Pore Range nm	% Volume	% SSA**
PET Coke*	Peak 1	0.35	0-0.38	8%	15%
	Peak 2	0.55	0.4-0.63	52%	68%
	Peak 3	0.82	0.66-1	11%	10%
	N2 Data		>1nm	29%	7%
	Total			100%	100%
Activated Peat Moss	Peak 1	0.35	0-0.38	4%	15%
	Peak 2	0.55	0.4-0.63	16%	40%
	Peak 3	0.82	0.66-1	9%	15%
	N2 Data		>1nm	71%	31%
	Total			100%	100%
Coconut Shell Carbon	Peak 1	0.35	0-0.38	4%	12%
	Peak 2	0.55	0.4-0.63	24%	44%
	Peak 3	0.82	0.66-1	16%	18%
	N2 Data		>1nm	56%	26%
	Total			100%	100%

Table 1: Surface characterization data of some carbon materials used in this study. *PET Coke is raw petroleum fluid coke. **SSA refers to specific surface area.

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