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Supercapacitors based on Carbon Nanotube Forests AJAY MURALIDHARAN, XINLI YOU, LAWRENCE PRATT, Tulane University, GARY HOFFMAN, Elizabethtown College —

Supercapacitors made of fibrous nano-materials have stirred the curiosity of the scientific community for the past three decades. Vertically aligned Carbon Nanotube forests (CNT) are excellent candidates for the supercapacitor electrode due to high surface area, tensile strength and electrical conductivity. Despite large efforts and rapid progress in developing CNT forests-based devices, our fundamental understanding of the underlying molecular mechanisms remain incomplete. We use molecular simulations to understand charging of CNT forests and the pore filling phenomena. The most serious uncertainty with previous simulations of CNT based supercapacitors was definition of the actual composition of the pores. We perform direct simulations of filling of these pores with a widely used electrolyte solution, tetra-ethylammonium tetra-fluoroborate in propylene carbonate, (TEABF4/PC). We choose several pore sizes and nanotube charges and compare our MD results with experimentally measured values for the same system(CNT/TEABF4/PC). The potentials and capacitances calculated using the Poisson equation are consistent with experimentally measured values. We discuss the role of pore sizes on the capacitance of these systems.

Ajay Muralidharan
Tulane University

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