

## **574g Molecular Simulation and Hydrodynamic Characterization of Water in Cnt's - Influence of Electric Fields on Wetting and Infiltration**

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Molecular simulations of stylized and actual CNT structures elucidate the interaction of water nanodroplets with the carbon surface and infiltration in the interior. The influence of electric fields upon wettability is studied with various surface charge distributions, first for a droplet spreading over the exterior of a CNT around which it is impaled. The equivalent surface energy and effective "contact angle" are characterized with continuum capillarity theory. Electric-field-driven penetration of water into tube mouths is demonstrated, and interior versus exterior wettability are compared. Schemes for controlling the nanoscale "meniscus" are explored.