

Abstract Submitted
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A Molecular Dynamics Study on the Exfoliation of Single Walled Carbon Nanotubes in Supercritical Carbon Dioxide¹ SEMRA SENTURK-OZER, Stevens Institute of Technology, DENIZ RENDE, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute — Carbon nanotubes (CNTs) could be used in various technological applications due to their structural, electrical and mechanical properties. However, in order to get the theoretically predicted benefits, nanotubes have to be successfully dispersed in the polymer matrix. Supercritical fluids were previously shown to result in good dispersion of nanofillers (in the case of clays and spherical nanofillers). In the current study, we investigated the potential use of supercritical carbon dioxide to unbundle single walled carbon nanotubes via molecular dynamics simulations. Various carbon nanotube systems were simulated with XenoView simulation software, and the effect of surface modification of nanotube with CO₂-philic chemicals was investigated on nanotube dispersion. Results showed that surface modification of nanotubes improves their dispersion in supercritical carbon dioxide.

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