

**MOLECULAR DYNAMICS STUDY OF  
SODIUM DODECYLBENZENE SULFONATE ADSORPTION ON  
SINGLE-WALLED CARBON NANOTUBES**



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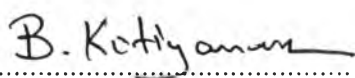
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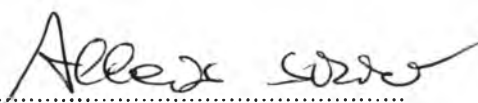
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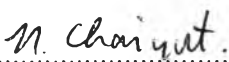
  
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## บทคัดย่อ

มนัสวี สุทธิพงษ์ : การศึกษาการดูดซับของสารลดแรงตึงผิวโซเดียมโดเดซิลเบนซีนซัลโฟเนตบนท่อคาร์บอนนาโนผนังชั้นเดียวโดยวิธีการจำลองเชิงโมเลกุล (Molecular Dynamics Study of Sodium Dodecylbenzene Sulfonate Adsorption on Single-Walled Carbon Nanotubes)  
 อ. ที่ปรึกษา : ผศ. ดร. บุญยรัชต์ กิตยานันท์ และ ผศ. ดร. แอลเบอร์โต สตรีโอโล 61 หน้า

การดัดแปลงพื้นผิวของท่อคาร์บอนนาโนผนังเดี่ยว (SWNTs) ด้วยกระบวนการดูดซับสารลดแรงตึงผิว (Surfactants) สามารถทำให้ท่อคาร์บอนนาโนกระจายตัวในน้ำและแยกออกจากกลุ่มมัดท่อคาร์บอนนาโน (SWNT bundles) ได้ แต่อย่างไรก็ตาม กลไกในระดับโมเลกุลของกระบวนการดูดซับสารลดแรงตึงผิวยังไม่เป็นที่แน่ชัด วิธีการจำลองเชิงโมเลกุล (Molecular dynamics simulations) ช่วยทำให้เข้าใจถึงโครงสร้างและพฤติกรรมการจัดเรียงตัวของสารลดแรงตึงผิวในระดับโมเลกุลได้ดีขึ้น ทั้งนี้ โครงสร้างการจัดเรียงตัวของสารลดแรงตึงผิวบนท่อคาร์บอนนาโนมีอิทธิพลต่อพลังงานแรงศักย์เฉลี่ย (Effective potential of mean force) ระหว่างคู่ท่อคาร์บอนนาโน งานวิจัยนี้ได้ศึกษาพฤติกรรมการจัดเรียงตัวในระดับโมเลกุลของสารลดแรงตึงผิวบนท่อคาร์บอนนาโนผนังเดี่ยวชนิดอาร์มแชร์ขนาด (6,6), (12,12), และ (20,20) โดยใช้วิธีการจำลองเชิงโมเลกุล ซึ่งในงานวิจัยนี้สารลดแรงตึงผิวโซเดียมโดเดซิลเบนซีนซัลโฟเนตปริมาณ 1.0 และ 2.8 โมเลกุลต่อพื้นที่ผิวท่อคาร์บอนนาโน อันประกอบด้วยหมู่วงแหวนเบนซีนซัลโฟเนตตำแหน่งที่ 5 หรือ 12 ของอะตอมคาร์บอนในสายโซ่โดเดซิลได้ถูกนำมาศึกษา จากผลการวิจัยพบว่า โครงสร้างโมเลกุลของสารลดแรงตึงผิวมีอิทธิพลต่อพฤติกรรมการจัดเรียงตัวของสารลดแรงตึงผิวบนท่อคาร์บอนนาโน ซึ่งสามารถนำไปใช้ระบุคุณสมบัติของสารลดแรงตึงผิวที่ควบคุมอันตรกิริยาระหว่างท่อคาร์บอนนาโนได้

**ABSTRACT**

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Stabilizing single-walled carbon nanotubes (SWNTs) monodispersed in diameter and chirality in aqueous media remains elusive. Surfactants have proven useful in deploying ultra-centrifugation techniques for separating carbon nanotubes, but the molecular mechanism responsible for the effectiveness for such technique remains not fully understood. Based on recent molecular simulation results, it appears that the morphology of self-assembled surfactant aggregates on carbon nanotubes strongly affects the effective potential of mean force between pairs of interacting carbon nanotubes. In the present work, the effect of surfactant molecular structure on the properties of aqueous surfactant self-assembled aggregates was investigated using all-atom molecular dynamics simulations. To quantify how the surfactant molecular structure affects self-assembly, sodium dodecylbenzene sulfonate (SDBS) surfactants with the headgroup located either on the fifth or on the twelfth carbon atom along the dodecyl tail were considered. All simulations were conducted at room conditions for different surface coverages on (6,6), (12,12), and (20,20) SWNTs. The results suggest that the surfactant molecular structure strongly affects the packing of surfactants on the nanotubes, therefore modulating effective nanotube-nanotube interactions. In qualitative agreement with experiments, no strong effects due to nanotube diameter were observed.

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