Modeling the Interaction Between Ethylene Diamine and Water Films on the Surface of a Carbon Nanotube

Richard L. Jaffe
NASA Ames Research Center
Moffett Field, CA 94035

Jens H. Walther, Urs Zimmerli and Petros Koumoutsakos
Institute of Computational Science
ETH
Zurich, CH-8092 Switzerland

It has been observed[1] that a carbon nanotube (CNT) AFM tip coated with ethylene diamine (EDA) penetrates the liquid water-air interface more easily than an uncoated nanotube tip. The EDA coating remains intact through repeated cycles of dipping and removal. In order to understand the physical basis for this observation, we use ab initio quantum chemistry calculations to study the EDA-CNT-water interaction and to parameterize a force field describing this system. Molecular dynamics (MD) simulations are carried out for EDA-water mixtures (figure 1) and an EDA-coated carbon nanotube immersed in water (figures 2 and 3). These simulations are similar to our earlier MD study[2] that characterized the CNT-water interface.

The attractive CNT-EDA and CNT-water interactions arise primarily from van der waals forces, and the EDA-EDA, EDA-water and water-water interactions are mainly due to hydrogen bond formation. The binding energy of a single EDA molecule to the nanotube is nearly three times larger than the corresponding value found for water (4.3 versus 1.5 kcal/mol, respectively). The EDA molecules readily stick to and diffuse along the CNT surface. As a result, mixing of the EDA and water films does not occur on the timescale of the MD simulations (figure 4). The EDA film reduces the hydrophobicity of the nanotube surface and acts like a prototypical surfactant in stabilizing the suspension of carbon nanotubes in water.

For this presentation, we use the MD simulations to determine how the presence of the carbon nanotube surface perturbs the properties of EDA-water mixtures.

References

[1] R. Stevens, C. Nguyen and M. Meyyappan; IEEE Trans. Nanobioscience **3**, 56 (2004).

[2] J Walther, R. Jaffe, T. Halicioglu and P. Koumoutsakos, J. Phys. Chem. B **105**, 9980 (2001).

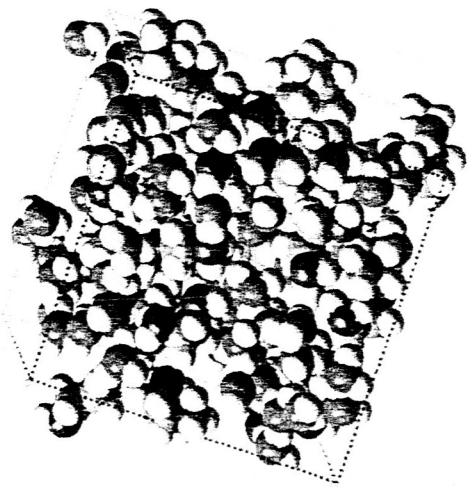


Figure 1: Snapshot from a MD simulation of a 1:2 EDA-water mixture. Red spheres represent water oxygen atoms, blue and gray spheres are EDA nitrogens and carbons, respectively, and white spheres are hydrogen atoms. Periodic boundary conditions are used and the dotted line displays the simulation cell.

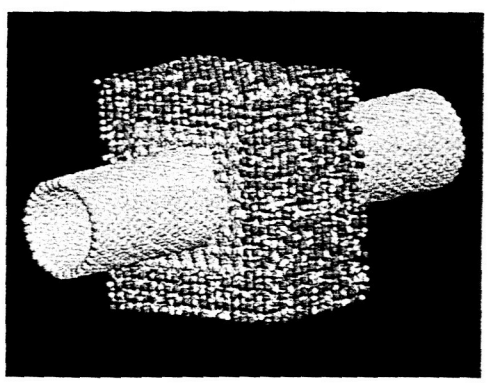
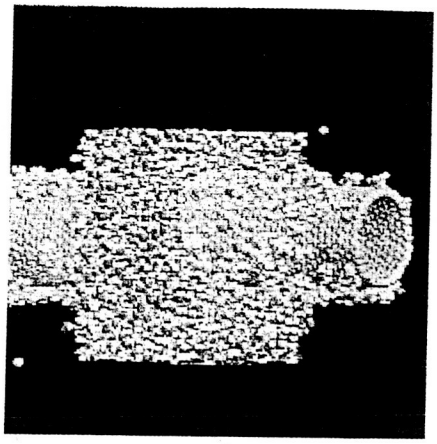


Figure 2: Initial configuration for the CNT-EDA-water MD simulation. Simulation cell has dimensions 14 X 6 X 6 nm and the water slab is 4 nm thick.

(A)



(B)

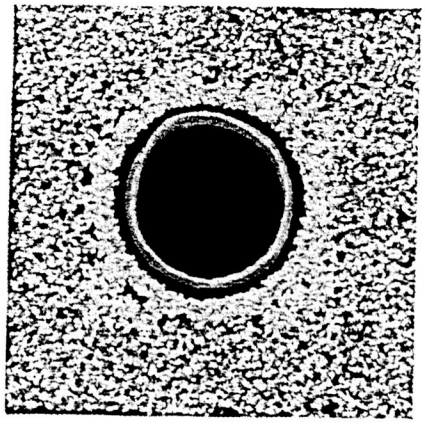


Figure 3: Two views from the CNT-EDA-water MD simulation after 300 ps. In (A), the physisorbed EDA layer is seen to have spread along the length of the nanotube without desorbing. In (B), it can be seen that there is no significant mixing of the EDA and water layers.

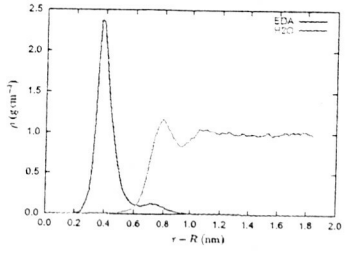


Figure 4: Radial densities of the EDA and water molecules in the CNT-EDA-water MD simulation. r – R is the normal distance of a liquid molecule from nanotube surface. The EDA density peak is at 4 Å and the first water peak is at 7.8 Å. The small overlap of the two curves indicates little mixing of EDA and water has occurred.