Surface Chemistry Research Laboratory

Head of Laboratory

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Research Plan

Surface Chemistry

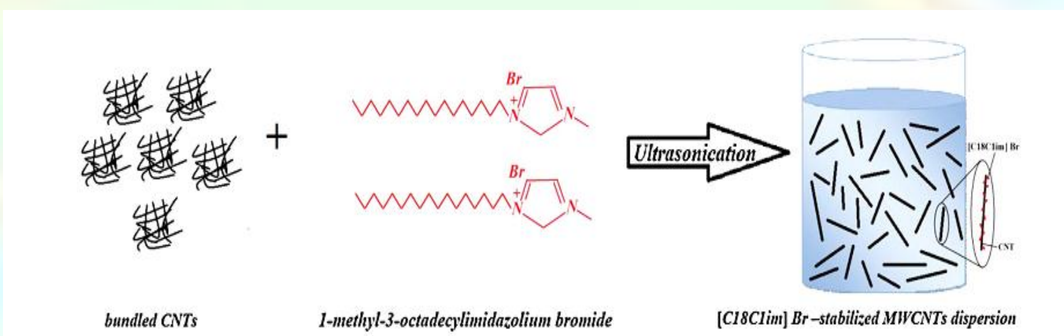
1-New energies

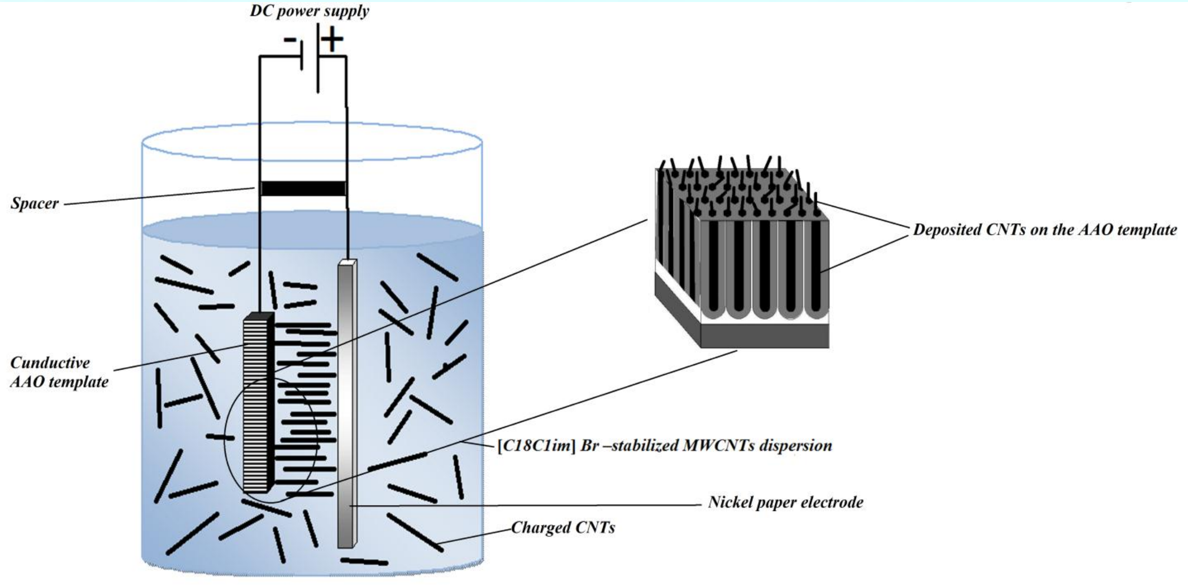
1-1.Supercapacitors:

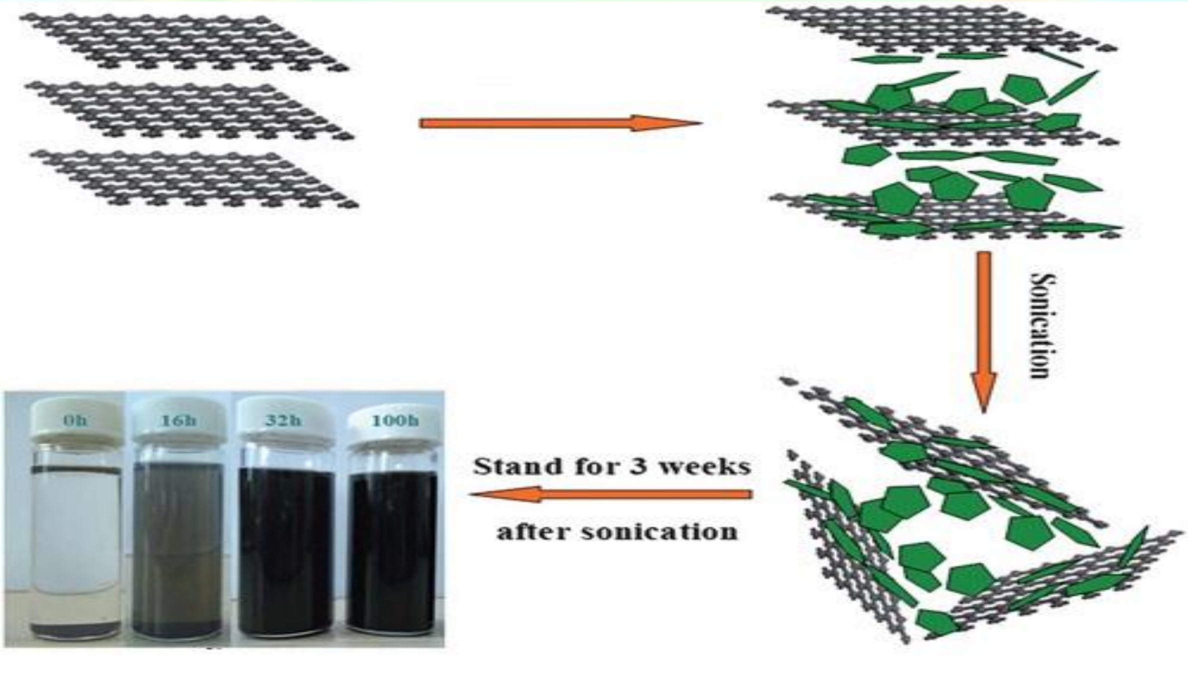
Today, with the growing concern over the use of fossil fuels, due to the risk of deficiency of these resources, a science movement is needed for energy production. Hence the need to develop methods for power reserve, restore it when needed, as well as felt. With increase in packing densities of integrated circuits, we need structures that can provide higher energy and power densities. Energy can be stored statically in electric fields instead of using chemicals to store energy chemically. The energy stored in this way can be extracted quickly and more efficiently. Electrical energy was stored as direct and indirect. In indirect method (in batteries), energy is produced by redox reactions between two electrode with various potentials. In direct method (in supercapacitors), energy is stored by physically separating positive and negative charges. Hence, an ionic layer is formed by the separation of positive and negative charges on the negative plate side. This accumulation of positive ions on one side leads to the accumulation of negative ions (electrons) on the other, positive electrode side. The charges are separated in this way, and energy is stored in these ionic double layers statically. Storing energy statically is fast and highly reversible. Thus, supercapacitors can be charged and discharged hundreds of thousands of times, leading to a longer life cycle. The energy storage and extraction are achieved through the movement of ions between the electrode surfaces. The charging and discharging of the supercapacitors are much faster than the extraction of energy from the chemical reactions taking place in batteries. Supercapacitors also have higher energy and power densities owing to high capacitance. Supercapacitors are constructed using materials with higher surface area that leads to higher capacitance.

1-1-1. Dispersion of carbon nanotubes and Grapheme as electrodes in supercapacitors:

Carbon nanotubes and Graphene are very important as an electrode material for supercapacitors. Due to the strong van der Waals tube-tube and sheet-sheet attraction and the hydrophobic property, they have extremely low solubility in most common solvents, which limit their applications in many fields. Uniform dispersions of CNTs and Graphene sheets in various solutions, especially in aqueous solution, are required. Different approaches have been developed to disperse CNTs and Graphene sheets through stirring and sonication methods. To disperse CNTs in water, the non-covalent method with aid of ionic liquid (IL) and surfactants are used. After dispersing CNTs by these materials, well dispersed CNTs are aligned on desired template by applying electric field. This technique, also called Electrophoretic deposition (EPD), is achieved via the motion of charged CNTs dispersed in IL, towards a conducting electrode under an applied electric field. The final goal is production of a film where most CNTs are aligned to certain direction. Electrophoretic motion of charged dispersed CNTs during EPD results in the accumulation of CNTs, which are encapsulate within an IL micelle, and formation of homogenous and rigid deposit at the relevant electrode.

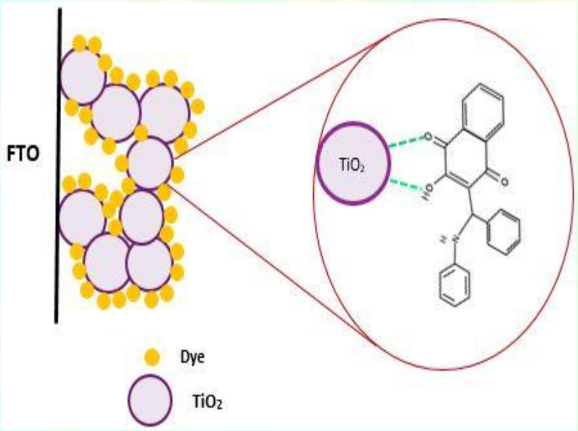


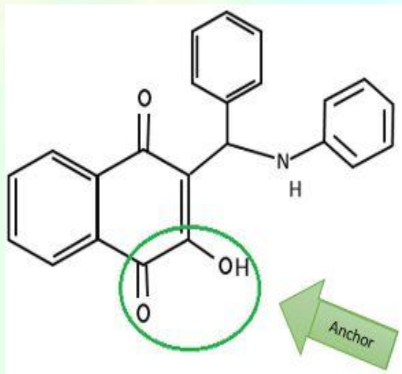

DC power supply
Spacer
Cunductive
AAO template
Deposited CNTs on the AAO template
[C18C1im] Br –stabilized MWCNTs dispersion
Nickel paper electrode
Charged CNTs

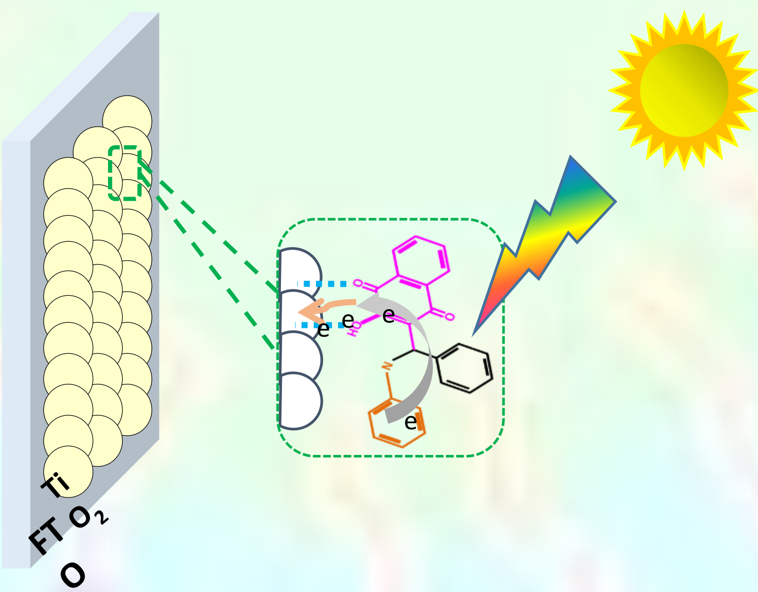

Sonication
Stand for 3 weeks
after sonication
0h
16h
32h
100h

1-2.Solar cells

Dye-sensitized solar cells (DSCs) have attracted intense interest due to their low cost and relatively high energy conversion efficiency. Organic dyes have several advantages such as larger absorption coefficients, change the substituents to easy control of their absorption and cell efficiency and not harmful to the environment. Therefore, we introduce the novel organic natural dye based on naphthoquinone derivative as a safe environment sensitizer for DSCs.





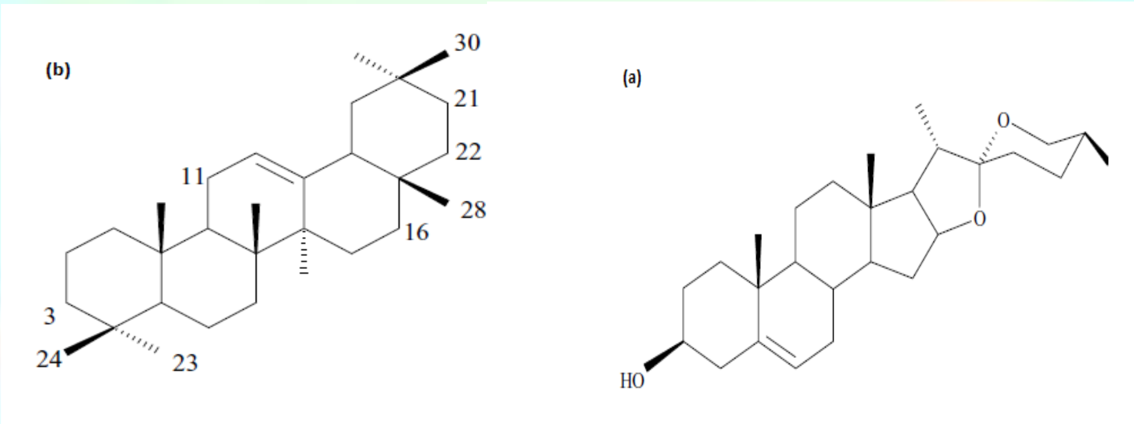


2-Natural and Magnetic surfactants

Environmental pollution is one the most important issue that has been investigated by environmental friendly scientists in recent years. Crude oil and its products such as light cycle oil (LCO), light gas oil (LGO) and heavy crude oil (CRU) are one of these pollutions. Chemists and chemical engineers are more interested in the collection methods, removing and cleanup of oil spills. Nowadays using of chemical agents such as dispersants are more employed to remove oil pollution of water to break down the crude oil into small droplets where natural processes can consume the oil spill over time.

2.1. Natural Surfactants

Natural surfactants benefit of environmentally compatibility and degradability comparing to their chemical counterparts. These materials are extracted from some plants in our laboratory.

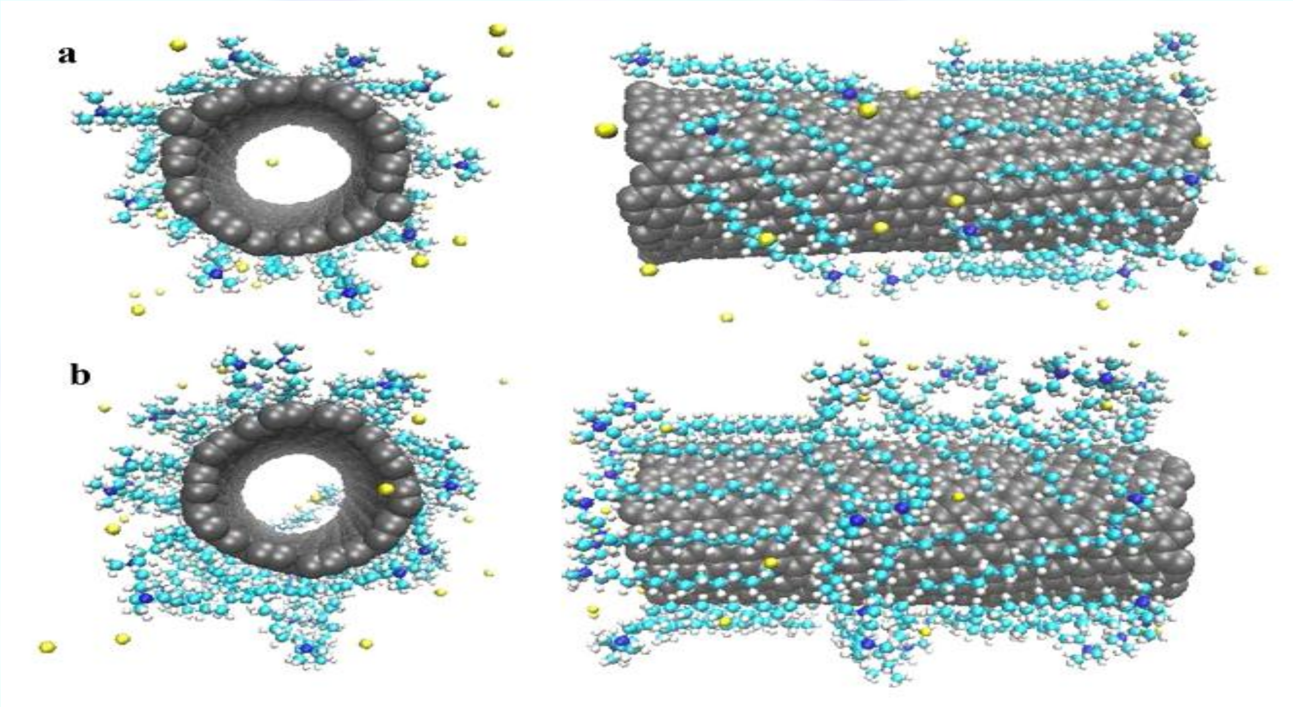


2.2. *Magnetic Surfactants*

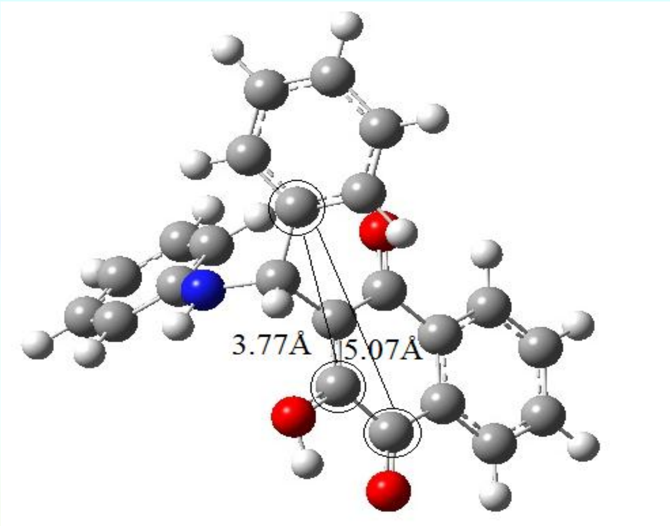
Magnetic surfactants may sound like a strange idea, but they have some very practical applications. For example, many surfactants are not biodegradable. If magnetic surfactants were used instead, they could be retrieved from waste-water using a magnetic field and recycled, resulting in lower levels of detergents entering the environment. Moreover, currently when there is an oil spill at sea, surfactants are used to break oil slicks into emulsion droplets so small that they diffuse away into the ocean, where the oil remains a pollution hazard. If magnetic surfactants were used instead, the resulting emulsions could be collected, removing both the oil and the surfactants from the water.

3-Simulation and quantum computational

The insolubility of carbon nanotubes (CNTs) and Graphite in aqueous media has been a limitation for the practical application of these unique materials. Recent studies have demonstrated that the suspendability of CNT (Graphene sheets) can be substantially improved by employing appropriate surfactants. Although various surfactants have been tested, the exact mechanism by which carbon



nanotubes and the different surfactants interact is not fully understood. To deepen the understanding of molecular interaction between CNT and surfactants, as well as to investigate the influence of the surfactant tail length on the adsorption process, we report here the first detailed large-scale all-atomistic molecular dynamics simulation study of the adsorption and morphology of aggregates of the cationic surfactants on single-walled carbon nanotube (SWNT) surfaces and Graphene sheet.



Research Subjects:

- Supercapacitors
- Dye synthesis solar cell
- Natural surfactants
- Magnetic surfactants
- Surfactant-CNT interaction
- Surfactant-Graphene interaction
- Remove oil pollution of water by surfactant

Experimental Methods

- Surface tension
- Conductometry
- PFG-NMR
- Dynamic light scattering
- Zeta potential
- Scan electron microscopy
- Transfer electron microscope
- Cyclic voltammetry
- Electrophoretic deposition
- Impedance

- Chemical vapor deposition
- Charge-discharge Galvanostatic
- Uv-visible spectrophotometry

Computational Methods

- Molecular Dynamic Simulation(MD)
- Density Functional Theory(DFT)
- Time Dependent Density Functional Theory(TD-DFT)

Instrumentals

UV-Vis Spectrophotometer mini Shimadzu 1240

Tensiometer Sigma 700

Sunny Simulator

Memmert Water Bath

Memmert Oven

Hot Plate 60

Sartorius TE124S Balance

Centrifuge Hettich EBA 270

Wise Circu

Wise Bath

Cyclic Voltammetry (Sama 500)

Computational System (12 core)

Conductometer Jenway

Research Publications

Supercapacitors

1.Electrophoretic deposition of multi-walled carbon nanotubes onporous anodic aluminum oxide using ionic liquid as a dispersing agent, F. Hekmat, B. Sohrabi, M.S. Rahmanifar, A. Jalali, Applied Surface Science 341 (2015) 109–119.

2.Supercapacitive properties of coiled carbon nanotubes directly grown on nickel nanowires, F. Hekmat, B. Sohrabi, M. S. Rahmanifar, Journal of material chemistry A, 2, (2014) 17446–17453.

3.Growth of the cobalt nanowires using AC electrochemical deposition on anodized Aluminum oxide templates, F. Hekmat, B. Sohrabi, M. S. Rahmanifar, J Nanostruct Chem (2014) 4:105, DOI 10.1007/s40097-014-0105-2.

Dispersion of CNT by using surfactants: Experimental and MD simulation

1-Dispersion of Carbon Nanotubes using Mixed Surfactants Experimental and Molecular Dynamics Simulation Studies, Beheshteh Sohrabi, Niaz Poorgholami-Bejarpasi, and Nahid Nayeri, Journal of physical chemistry B, 118 (2014) 3094−3103.

2-Self-Assembly of Cationic Surfactants on the Carbon Nanotube Surface: Insights from Molecular Dynamics Simulations, N. Poorgholami, B. Sohrabi, Journal of molecular modeling, (2013) DOI: 10.1007/s00894-013-1948-z.

3-Role of surfactant structure in aqueous dispersions of carbon nanotubes Original N. Poorgholami-Bejarpasi, B. Sohrabi 2015, 394, 19-28

Surfactant interactions

1-Electrolyte-Cosolvent Simultaneous Effects on Adsorption and the Phase Transition between Microstructures and Nanostructures in the Cationic-rich Region of Catanionic Mixture, B. Sohrabi, M. Moallemi, R. Amani, M. Kiasadegh, Fluid phase equilibria, 375 (2014) 168-175.

2-Polymer-Surfactant Interaction in Catanionic surfactant Mixtures and its Application in Nanoporous Pores Synthesis, Colloid and surface, 436 (2013) 890-897. B. Tajik, B. Sohrabi, R. Amani.

3-Investigation of DNA-Cationic Bolaform Surfactants Interaction with Different Spacer Length, Colloids and surfaces B, 110 (2013) 29-35. V. Khani, B. Sohrabi, A. A. Mosavi Movahedi, P. Moradi.

4-Adsorption and micellar phase properties of anionic surfactant in the presence of electrolyte and oil at different temperatures, Fluid Phase Equilibria 337 (2013) 370–378. B. Sohrabi, P. Moradi, M. Najafi.

5-The study of Sunset Yellow anionic dye interaction with gemini and conventional cationic surfactants in aqueous solution, Dyes and Pigments 95 (2012) 768–775. Sara Fazeli, Beheshteh Sohrabi, Alireza Tehranibagha.

6-Electrolyte Effect on Adsorption and the Phase Transition from Microstructures to Nanostructures in Ionic/Ionic Surfactants Mixture, Journal of Colloid and Interface Science 361 (2011) 159–169. Maryam Moallemi, Beheshteh Sohrabi, Sara Fazeli.

7- The Electrolyte Effect on Nanostructures of Mixed Anionic and Cationic Surfactants, journal of nanostructure in chemistry, 2 (2011), 183-188. Maryam moallemi, Beheshteh Sohrabi.

8-Investigation of the mixing behavior of surfactants by the lattice Monte carlo simulation, J Mol Model (2010) 16:1499–1508. N. B. Poorgholami, S. M. Hashemianzadeh, B. Sohrabi