



NANOTECH FRANCE 2016

International Nanotechnology Conference
1 - 3 June 2016

Pôle Universitaire Léonard de Vinci, La Défense
Paris - France

Organizer



In Collaboration with



Joint Conference



09:30-09:45	Decontamination of wastewater using nanocarbon compounds insert in diatomite mesoporous structure E. Flores, O. Enriquez, J. De la Cruz, A. López, G.Poma and M.Quintana	Dr. Maria Quintana , Engineering and Technological University, Lima - Peru
09:45-10:00	Functionalization of glassy carbon electrode by amines electrochemical oxidation for micro-pollutants detection in water D. Pally, M. Alaaeddine, B. Cagnon, V. Bertagna , R. Benoit, F. Podvorica and C. Vautrin	Dr. Valerie Bertagna , University of Orleans - France
10:00-10:30 Coffee Break / Exhibition		
10:30-11:00	PVDF UF hollow-fiber membrane production as pre-treatment system in Water Desalination Reverse Osmosis Unit A. Figoli , O. Saoncella, S. Xue, S. Simone, F.Galiano, M. Boerrigter, C. Chaumette, M. Faccini and E. Drioli	Dr. Alberto Figoli , Institute on Membrane Technology (CNR-ITM) - Italy
11:00-11:15	Development of Alumina-Carbon Nanotubes Porous Membranes Using Spark Plasma Sintering Process for Water Purification T. Laoui , H. K. Shahzad, M. A. Hussein, F. Patel, N. Al Aqeeli and M. A. Atieh	Prof. Tahar Laoui , King Fahd University of Petroleum and Minerals- Saudi Arabia
11:15-11:30	The efficient separation of oil-water emulsions with a flexible, superhydrophilic and self-cleaning TiO ₂ /Fe ₂ O ₃ membrane B.Y.L. Tana , J. Juaya, J.K.K. Anga, Z.Liub and D. Suna	Mr. Benny Tan , Nanyang Technological University - Singapore
11:30-11:45	Nanostructure formation, characterization and application of ba-nana peels nanosorbent in mine water treatment O. Atiba-Oyewo , M.S. Onyango and C. Wolkersdorfer	Ms. Opeyemi Atiba-Oyewo , Tshwane University of Technology - South Africa
11:45-12:00	Fabrication of hematite photoanode for solar water splitting by using pulsed laser deposition C-P.Yen , Y-J. Li, S-J. Luo, J.Wang, C-J.Tseng and S-Y Chen	Mr. Chih-ping Yen , National Taiwan University - Taiwan
12:00-12:15	Molecular Dynamics-Continuum Hybrid Simulation of Water Transport through Carbon Nanotube Membranes A. Kudaikulov , A. Kaltayev and C. Jossierand	Mr. Aziz Kudaikulov , Al-Farabi Kazakh National University - Kazakhstan
12:15-12:30	Titanium Dioxide-Based Nanocatalysts Constructed from Natural Sources for Photocatalytic Wastewater Treatment P. Kемacheevakul and S.Chuangchote	Dr. Patiya Kемacheevakul , King Mongkut's University of Technology - Thailand
12:30-12:45	Magnetic Nanoparticles Stabilized by Lignocellulosic Waste as Green Adsorbent For Cr(VI) Removal from Waste Water I.L.A. Ouma , A.E. Ofomaja and E.B. Naidoo,	Ms. Linda Ouma , Vaal University of Technology-South Africa

Posters Session II: June 2nd, 2016

NanoMatEn 2016

Exhibition and Poster Hall

N.	Title	Author/Affiliation/Country
1	Solar charged redox flow battery K. Wedege , J. Azevedo, A. Khataee, A. Mendes and A. Bentien	Ms. Kristina Wedege , Aarhus University - Denmark
2	Novel Methods for the Deposition of Solution-Processed CdTe Inks for Photovoltaic Applications J.C. Russell , J.M. Kurley, H. Zhang and D. Talapin	Mr Jake Russell , University of Chicago - USA
3	Enhancement of power conversion efficiency of dye-sensitized solar cells via incorporation of GaN semiconductor materials synthesized in hot-wall CVD furnace. M. Baisariyev , R.Iskakov, G. Sugurbekova	Mr. Murat Baisariyev , Nazarbayev University - Kazakhstan

Molecular Dynamics-Continuum Hybrid Simulation of Water Transport through Carbon Nanotube Membranes

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Abstract:

Nanotechnology holds great potential in advancing water and wastewater treatment to improve treatment efficiency as well as to augment water supply through safe use of unconventional water sources. Various types of nanomaterials, such as nanoadsorbents, nanometals, nanomembranes, and photocatalysts, have been utilized in water treatment applications. However, the prediction of the fluid mass flow rate and heat transfer in nanoscale systems presents a major barrier to their design. The existence of non-continuum effects, such as molecular layering and velocity slip near to liquid–solid interfaces, seemingly precludes efficient continuum computational fluid dynamics (CFD). On the other hand, more accurate molecular dynamics (MD) simulations can be extremely costly in terms of the computational resources they require. In this paper we used the molecular dynamics-continuum hybrid simulation to investigate the water transport through carbon nanotube (CNT) membranes (Figure 1). We present a procedure for using molecular dynamics (MD) simulations to provide essential fluid and interface properties for subsequent use in computational fluid dynamics (CFD) calculations of nanoscale fluid flows. Comparison with full-scale MD simulations demonstrate that these enhanced CFD simulations providing good flow field results in a range of complex geometries at the nanoscale.

Keywords: computational fluid dynamics, molecular dynamics, hybrid methods, carbon nanotube membranes, non-continuum effects, molecular layer, slip flow.

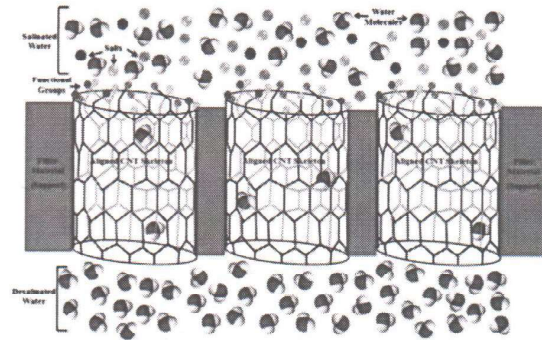


Figure 1: Carbon nanotube membranes (CNT).

References:

David, M., Duncan, A., Matthew, K., William, D., Jason, M. (2015) Molecular dynamics pre-simulations for nanoscale computational fluid dynamics, *Microfluidics and Nanofluidics*, Volume 18, Issue 3, 461-474.

Xiaolei, Q., Pedro, J., Qilin, L. (2013), Applications of nanotechnology in water and wastewater treatment, *Water Research*, Volume 47, Issue 12, 3931-3946.