SAND2017-4936R

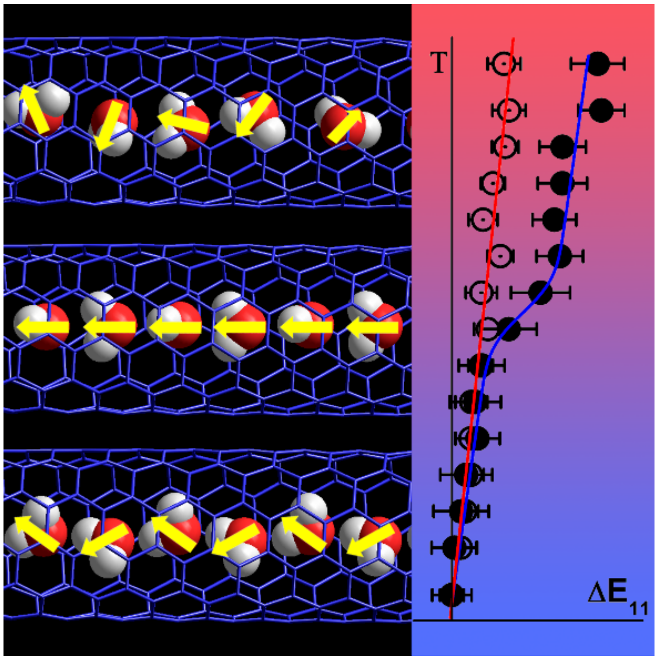
CINT Report to BES/SUFD
May 5, 2017

High-Impact Science Highlights (Slides and original papers are attached)

Does nano-water "freeze" at 150 K?

Category: *Enablers*

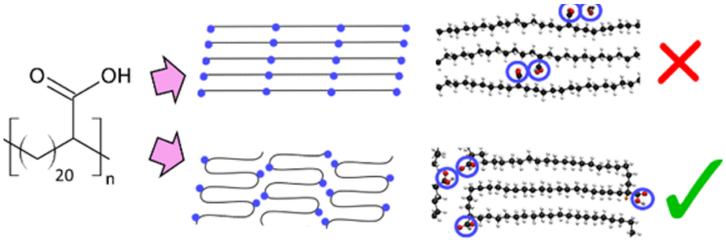
Nanoconfined water plays important roles in many natural phenomena and has potential to be exploited for technological applications, such as water desalination or targeted drug delivery. In a joint effort of the Center of Integrated Nanotechnologies and the University of Antwerp (Belgium), the temperature-dependent behavior of a single molecular array of water molecules has been investigated. To this end, Xuedan Ma and colleagues encapsulated water molecules inside ultrathin carbon nanotubes, with a diameter just able to fit one single row of water molecules. The authors found an unexpected temperature-induced transition in the orientation of the water dipoles, which could be detected as a change in the emission spectrum of the filled nanotubes. This is surprising considering Ising's paradigm that no phase transitions can occur in one-dimension. The authors support their findings with molecular dynamics simulations, and evidence the alignment of the dipole of all molecules in the same direction. This discovery is encouraging for the development of nanofluidics applications, such as ultra-selective purification, single-file proton transport channels, and mimicking biological membranes because the transport rate will strongly depend on the configuration of dipole orientations. On the right of the figure is the measured photoluminescence peak position as a function of temperature, with filled circles for water-filled nanotubes and open circles for empty nanotubes. The observed shift occurs when the water-filled nanotubes are cooled to ~150K. The left side of the figure shows a schematic of random and oriented water molecules (red and white) within carbon nanotubes (blue cage). The article, "Quasiphase Transition in a Single File of Water Molecules Encapsulated in (6,5) Carbon Nanotubes Observed by Temperature-Dependent Photoluminescence Spectroscopy," was published in *Physical Review Letters* [PRL **118,** 027402 (2017)].

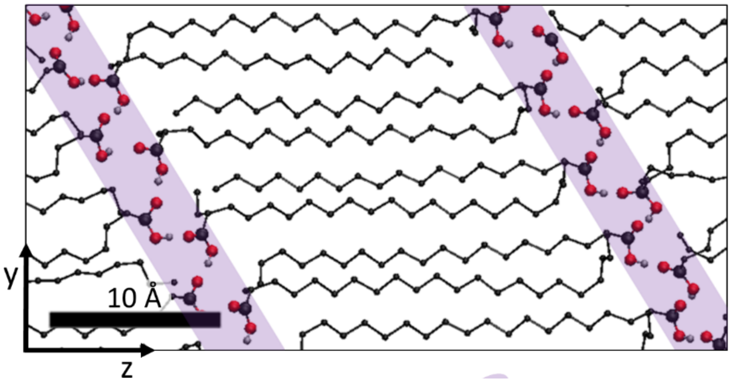


Novel Layered Polymer Crystal for Improved Transport

Category: *Enablers, Storage*

Ionomers are polymers with specific functional groups placed periodically along their carbon backbone. Membranes of these materials have interesting thermal and ion transport properties making them candidate electrolytes for energy storage devices. While most ionomers are amorphous and have relatively limited ion conductivity, by precisely controlling the polymer architecture, semicrystalline versions of these materials can be made that exhibit improved ion, proton, or small molecule transport properties. In work recently published in the Journal of the American Chemical Society, *J. Am. Chem. Soc.* (**139**, 3747−3755, 2017), the structure of a semicrystalline, precisely functionalized (carboxylic acid) polyethylene was studied by x-ray scattering, Raman spectroscopy, and molecular dynamics simulations. The molecular structure of this material is characterized by polymer chains that are folded back on themselves in a hairpin at every carboxylic acid group (colored atoms), as detailed in the lower figure, which is a representation taken directly from simulation results. This folding and alignment of the functional groups creates channels that act as a two-dimensional pathway where ion conduction is not hindered by the polymer chain (black atoms). By changing the choice of functional group, it should be possible to further optimize the transport properties for specific applications.





Scientific Leadership:

Dale Huber, CINT SBCN scientist, was issued US Patent 20160030920 - Programmable pH Buffers. A programmable pH buffer comprises a copolymer that changes pKa at a lower critical solution temperature (LCST) in water. The copolymer comprises a thermally programmable polymer that undergoes a hydrophobic-to-hydrophilic phase change at the LCST and an electrolytic polymer that exhibits acid-base properties that are responsive to the phase change. The programmable pH buffer can be used to sequester CO2 into water.

CINT undergraduate, **Randy Ko**, was selected for as a Goldwater Scholar. The Barry M. Goldwater Scholarship and Excellence in Education Program was established by the United States Congress in 1986 in honor of former United States Senator and 1964 presidential candidate Barry Goldwater, a Republican from Arizona. Its goal is to provide a continuing source of highly qualified scientists, mathematicians, and engineers by awarding scholarships to college students who intend to pursue careers in these fields.

Long time CINT user, **Ron Salesky** (The University of New Mexico), has successfully defended his PhD thesis (DNA directed assembly of gold-tipped metallic single-walled carbon nanotubes into electrical devices). Much of the work in his thesis was work done using CINT facilities. CINT SBCN scientist, **Jennifer Martinez** was one of his mentors for his thesis and served on his committee.
Ryan Camacho, CINT NPON scientist, was invited to address the Department of Energy's National Science Bowl. During the opening event, he gave a talk titled, "Diamonds aren't forever: How atomic imperfections could be the key to quantum engineering." The theme this year was Quantum Information Science, and Ryan's work was featured on the cover of the Science Day booklet.

Nate Mara, CINT NEM scientist, received a Young Researcher award from the *International Journal of Plasticity*. The award honors his contributions to the field of plasticity, especially modeling plastic deformation and the mechanics of metals and nanocomposites. Mara received the award at the 2017 International Symposium on Plasticity and its Current Applications. *The International Journal of Plasticity* selects the Young Researcher Award recipients based on a combination of publication citations, service to the journal and overall quality of research, and impact on the deformation plasticity field.

User Program & Outreach:

CINT received 210 proposal submission in its Spring call for proposals held March 1-31, 2017. This is CINT's largest number of proposal submissions in a single call since its inception. Data collected on submissions show that increased outreach efforts by our scientists and staff contributed significantly to this increase. 73% of the proposals submission were new while 27% were continuation proposals. Academic institutions made up 53% of the total submissions, 34% were internal laboratory submissions, 6% were from Industry and 7% other agencies.

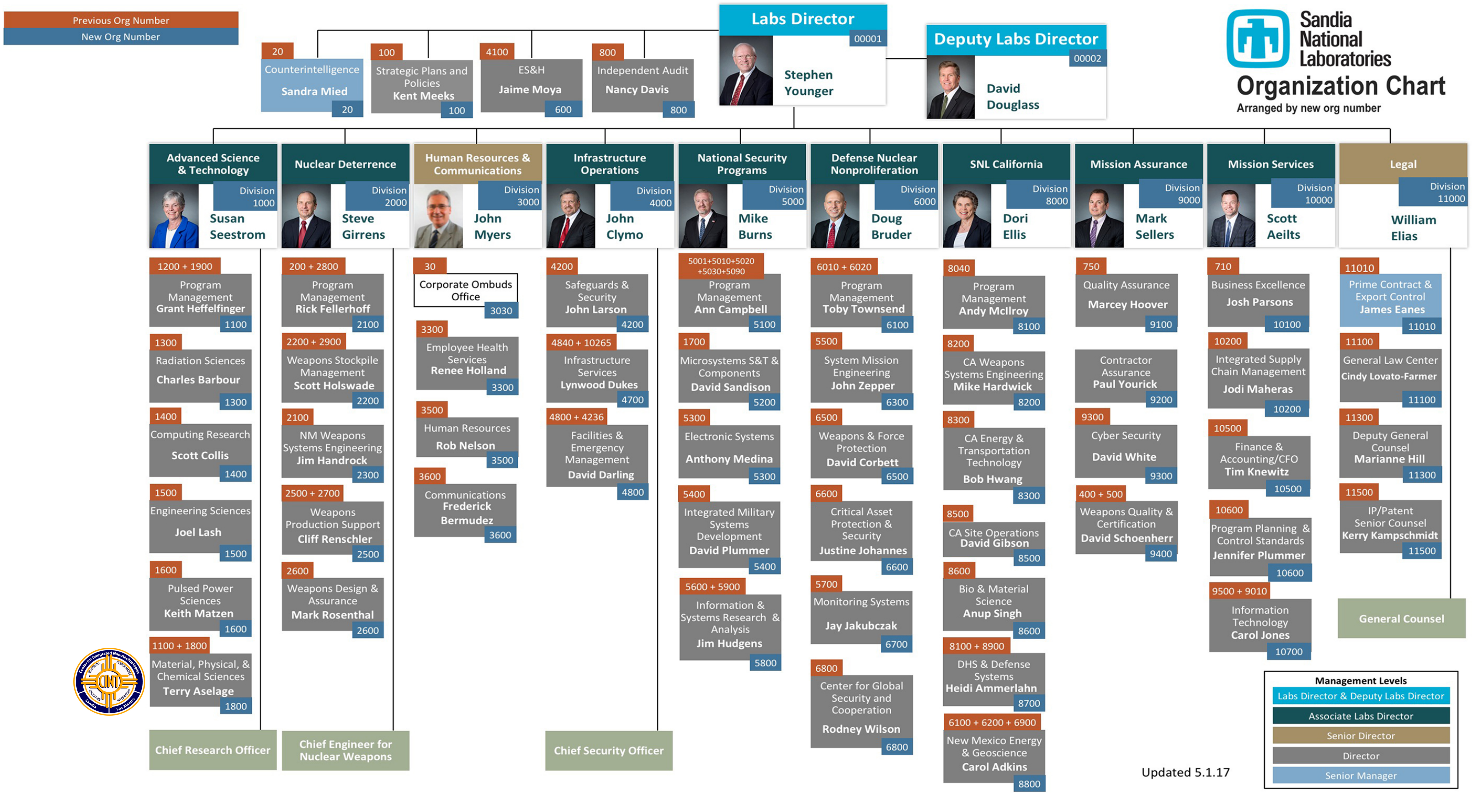
CINT's Annual meeting will be held on September 25-26, 2017 at the La Fonda hotel in Santa Fe, NM. The meeting will feature three concurrent symposia focused on Quantum Materials Integration, Soft Matter and Microscopy. The meeting will feature two satellite events, a TEM training session being held on Sept 24th and a joint NSRC theory session extending through the meeting to the afternoon of the 27th.

News:

It is our great pleasure to announce that **Dr. Andreas Roelofs** will be joining LANL as CINT Director and LANL CINT Group Leader. Andreas will be joining us from Argonne National Laboratory (ANL), where he currently is the Director of the Laboratory's Lab-Embedded Entrepreneurship Program Chain Reaction Innovations (CRI) and the Nano Design Works (NDW) center. He previously served as Deputy and later as interim Director of both the Nanoscience and Technology Division and the Center for Nanoscale Materials (CNM), CINT's counterpart at ANL. Andreas's technical expertise is in ferroelectric thin films and nanoparticles for ferroelectric random access memory. He holds a doctoral degree in physics with highest honors from the RWTH Aachen in Germany and is the author of 47 peer-reviewed publications and 15 patents. We are equally delighted to announce that **Dr. Sean Hearne** from Sandia National Laboratories will assume the role of CINT Co-Director. Grant will remain Acting CINT Director until Andreas's arrival as Director at which time Sean Hearne will become Co-Director

CINT held an All-Hands meeting at Los Alamos on April 11. Approximately 60 scientists, research technologists, and administrators gathered to hear a number of important CINT-related updates. These updates included CINT leadership transitions and the current status of the search for a CINT Director/co-Director to be located at the Gateway Facility in Los Alamos. New hires were introduced as well as an announcement of five new SAC members. Additionally, Sean Hearne updated the group about progress towards triennial review milestones. There were vibrant discussions in small groups over lunch about the ways the annual CINT user meeting could be improved, with some of the more facile changes to be implemented for the next CINT Annual Meeting. Finally, there were two strategy presentations on Quantum Materials and the Brain Initiative before scientists broke up into separate Thrusts to discuss thrust-specific business.

On May 1, the National Technology & Engineering Solutions of Sandia (NTESS) took over management and operations of Sandia National Laboratories. Due to this change, current Acting CINT Director, **Grant Heffelfinger**, will be moving to a new role at Sandia, Director for Program Management, Advance S&T. He will also serve as deputy to the laboratory's Chief Research Officer, **Susan Seestrom**, who will also lead the 1000 Directorate as Associate Laboratory Director for Advance Science & Technology. The CINT organization will now be under the Material, Physical, & Chemical Sciences Center, led by **Terry Aselage**. Terry will assume the Sandia role on the CINT Executive Management Team.



Sandia National Laboratories

Organization Chart

Arranged by new org number

Previous Org Number

New Org Number

Labs Director 00001

Stephen Younger

Deputy Labs Director 00002

David Douglass

Previous Org Number		New Org Number
20	Counterintelligence **Sandra Mied**	20
100	Strategic Plans and Policies **Kent Meeks**	100
4100	ES&H **Jaime Moya**	600
800	Independent Audit **Nancy Davis**	800

Advanced Science & Technology

Division 1000

Susan Seestrom

Previous Org Number		New Org Number
1200 + 1900	Program Management **Grant Heffelfinger**	1100
1300	Radiation Sciences **Charles Barbour**	1300
1400	Computing Research **Scott Collis**	1400
1500	Engineering Sciences **Joel Lash**	1500
1600	Pulsed Power Sciences **Keith Matzen**	1600
1100 + 1800	Material, Physical, & Chemical Sciences **Terry Aselage**	1800

Chief Research Officer

Nuclear Deterrence

Division 2000

Steve Girrens

Previous Org Number		New Org Number
200 + 2800	Program Management **Rick Fellerhoff**	2100
2200 + 2900	Weapons Stockpile Management **Scott Holswade**	2200
2100	NM Weapons Systems Engineering **Jim Handrock**	2300
2500 + 2700	Weapons Production Support **Cliff Renschler**	2500
2600	Weapons Design & Assurance **Mark Rosenthal**	2600

Chief Engineer for Nuclear Weapons

Human Resources & Communications

Division 3000

John Myers

Previous Org Number		New Org Number
30	Corporate Ombuds Office	3030
3300	Employee Health Services **Renee Holland**	3300
3500	Human Resources **Rob Nelson**	3500
3600	Communications **Frederick Bermudez**	3600

Infrastructure Operations

Division 4000

John Clymo

Previous Org Number		New Org Number
4200	Safeguards & Security **John Larson**	4200
4840 + 10265	Infrastructure Services **Lynwood Dukes**	4700
4800 + 4236	Facilities & Emergency Management **David Darling**	4800

Chief Security Officer

National Security Programs

Division 5000

Mike Burns

Previous Org Number		New Org Number
5001+5010+5020 +5030+5090	Program Management **Ann Campbell**	5100
1700	Microsystems S&T & Components **David Sandison**	5200
5300	Electronic Systems **Anthony Medina**	5300
5400	Integrated Military Systems Development **David Plummer**	5400
5600 + 5900	Information & Systems Research & Analysis **Jim Hudgens**	5800

Defense Nuclear Nonproliferation

Division 6000

Doug Bruder

Previous Org Number		New Org Number
6010 + 6020	Program Management **Toby Townsend**	6100
5500	System Mission Engineering **John Zepper**	6300
6500	Weapons & Force Protection **David Corbett**	6500
6600	Critical Asset Protection & Security **Justine Johannes**	6600
5700	Monitoring Systems **Jay Jakubczak**	6700
6800	Center for Global Security and Cooperation **Rodney Wilson**	6800

SNL California

Division 8000

Dori Ellis

Previous Org Number		New Org Number
8040	Program Management **Andy McIlroy**	8100
8200	CA Weapons Systems Engineering **Mike Hardwick**	8200
8300	CA Energy & Transportation Technology **Bob Hwang**	8300
8500	CA Site Operations **David Gibson**	8500
8600	Bio & Material Science **Anup Singh**	8600
8100 + 8900	DHS & Defense Systems **Heidi Ammerlahn**	8700
6100 + 6200 + 6900	New Mexico Energy & Geoscience **Carol Adkins**	8800

Mission Assurance

Division 9000

Mark Sellers

Previous Org Number		New Org Number
750	Quality Assurance **Marcey Hoover**	9100
	Contractor Assurance **Paul Yourick**	9200
9300	Cyber Security **David White**	9300
400 + 500	Weapons Quality & Certification **David Schoenherr**	9400

Mission Services

Division 10000

Scott Aeilts

Previous Org Number		New Org Number
710	Business Excellence **Josh Parsons**	10100
10200	Integrated Supply Chain Management **Jodi Maheras**	10200
10500	Finance & Accounting/CFO **Tim Knewitz**	10500
10600	Program Planning & Control Standards **Jennifer Plummer**	10600
9500 + 9010	Information Technology **Carol Jones**	10700

Legal

Division 11000

William Elias

Previous Org Number		New Org Number
11010	Prime Contract & Export Control **James Eanes**	11010
11100	General Law Center **Cindy Lovato-Farmer**	11100
11300	Deputy General Counsel **Marianne Hill**	11300
11500	IP/Patent Senior Counsel **Kerry Kampschmidt**	11500

General Counsel

Updated 5.1.17

Management Levels

- Labs Director & Deputy Labs Director
- Associate Labs Director
- Senior Director
- Director
- Senior Manager

Budget

I. Please see attached NSRC_CINT_Monthly_Budget_May_2017.xlsx for 1-yr projections and March 2017 monthly breakdown.

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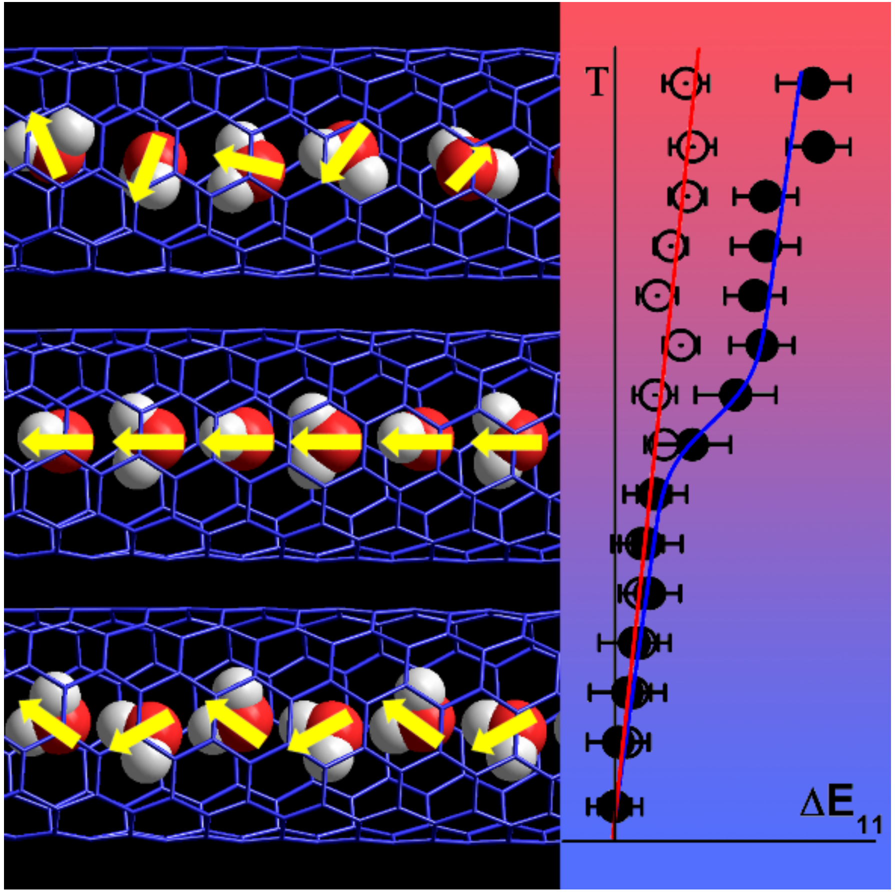
Does 1-D Nano-Confined Water Freeze at 150 K?

A Step Toward New Filtration and Drug Delivery Technologies

Category: *Enablers & Cross-cutting*



Water molecules (red and white balls) forming a chain in a carbon nanotube (blue lattice) normally orient randomly (yellow arrows; top and bottom left). Molecules align unexpectedly at 150°K (middle, left) and caused a sudden shift in the emission color (right, black data points). Emission color of an empty nanotube only shows gradual shift. (empty data points)

Scientific Achievement

An unexpected shift from random to ordered arrangement in orientation of dipoles (quasi-phase shift) is observed in a chain of water molecules encapsulated in a nanotube as they are cooled down to cryogenic temperatures.

Significance and Impact

Phase transition in one-dimensional system is of great fundamental physics interest. It is also a step closer to controlling fluid transport at the nanoscale for ultra-selective purification and drug delivery.

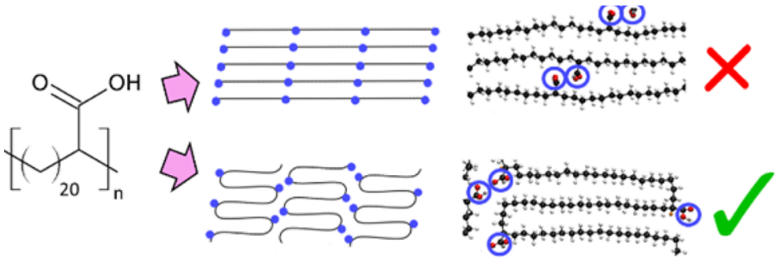
Research Details

- Photoluminescence from nanotubes filled with water was investigated as the function of temperature.
- A fairly sharp change in emission color was observed at 150 K.
- Molecular dynamics simulations attribute the change to a temperature-induced transition in the orientation of the water dipoles.

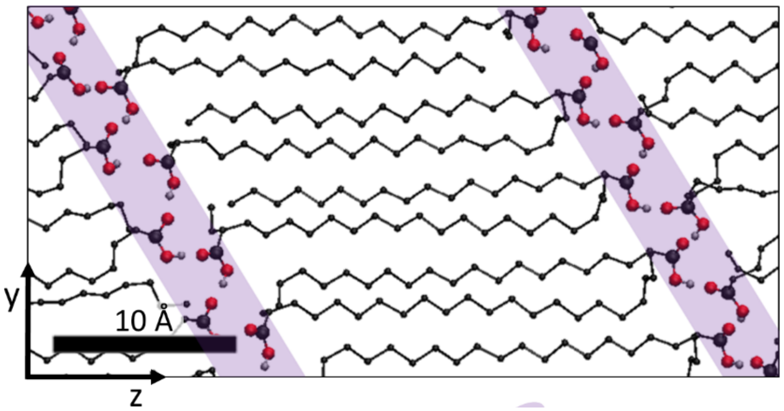
X. Ma, S. Cambré, W. Wenseleers, S. K. Doorn, H. Htoon , *Physical Review Letters*, **2017**, *118*, 027402. (Editor's Suggestion)
http://physicsworld.com/cws/article/news/2017/jan/23/quasi-phase-transition-spotted-in-water-filled-carbon-nanotubes

Work was performed at CINT and University of Antwerp, Belgium

Novel Layered Polymer Crystal for Improved Transport



A polymer with precisely spaced functional groups forms a new crystal structure with acid groups (-COOH) assembled in layers and novel hairpin turns of the polymer; see schematic (above) and detail from simulations (below). In image below, polyethylene backbone is shown as lines connecting dots and the acid group are highlighted in purple.



E. B. Trigg, M. J. Stevens, and K. I. Winey, *J. Am. Chem. Soc.*, **2017**. DOI: 10.1021/jacs.6b12817

Work was performed at CINT and U. Pennsylvania.

Scientific Achievement

Discovered a new crystalline structure in a precisely-functionalized polyethylene that has layers of acid groups just 2.5 nm apart.

Significance and Impact

This new morphology is expected to exist for a wide range of functional groups and, depending on the chemistry of the functional group, to provide faster proton, ion, or molecular transport in a solid polymer for a variety of potential energy-related applications.

Research Details

- By combining molecular dynamics simulations with experimental X-ray scattering and Raman spectroscopy data, we find that the polymer chains are folded in hairpins at each acid group to form layers of functional groups.
- This result contrasts with other precise polyethylenes with methyl or halide groups, wherein the polymer chains are straight within the crystals.
- E.B. Trigg was a DOE SCGSR fellow in summer 2014 at CINT .