Argonne NATIONAL LABORATORY 75 1946–2021

X-RAY SCIENCE DIVISION UPDATE

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PSC All Hands Meeting
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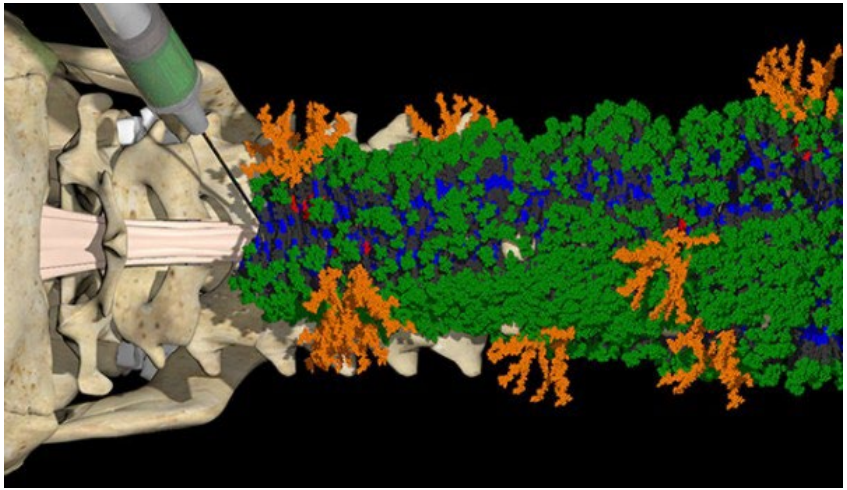
“DANCING MOLECULES” SUCCESSFULLY REPAIR SEVERE SPINAL CORD INJURIES

- Fine-tuning “dancing molecules’” motion within a nanofiber scaffold network makes them more agile, results in greater efficacy to reverse paralysis, repair tissue after severe spinal cord injuries
- Synchrotron solution x-ray scattering at DuPont-Northwestern-Dow Collaborative Access Team was used to understand scaffold morphology



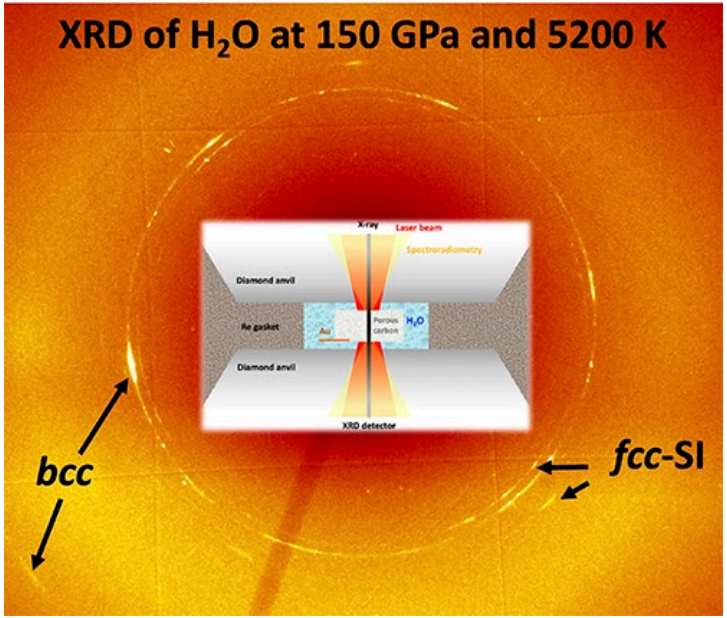
A new, injectable therapy forms nanofibers with two different bioactive signals (green and orange) that communicate with cells to initiate repair of the injured spinal cord - Illustration by Mark Seniw

Z. Álvarez, A.N. Kolberg-Edelbrock, I.R. Sasselli J.A. Ortega, R. Qiu, Z. Syrgiannis, P.A. Mirau, F. Chen, S.M. Chin, S. Weigand, E. Kiskinis, S. I. Stupp, ”Bioactive scaffolds with enhanced supramolecular motion promote recovery from spinal cord injury,” Science **374**, 848 (12 November 2021). DOI: 10.1126/science.abh3602

HOW DO ICE GIANTS MAINTAIN THEIR MAGNETIC FIELDS?

- A layer of “hot,” electrically conductive ice could be responsible for generating magnetic fields of ice giant planets like Uranus and Neptune
- DAC and XRD studies at GeoSoilEnviroCARS 13-ID revealed the conditions under which two such superionic ices form
- A few thousand experiments over a decade yielded high-quality

V. B. Prakapenka, N. Holtgrewe, S.S. Lobanov, A.F. Goncharov, “Structure and properties of two superionic ice phases,” Nat. Phys., published on line 14 October 2021. DOI: 10.1038/s41567-021-01351-8



The figure illustrates how the experiments were performed, revealing two forms of superionic ice. Image courtesy of Vitali Prakapenka (The University of Chicago)

FIRST USE OF THE NEW ALCF POLARIS TESTBED DURING APS BEAM TIME

Integration of 8-ID-I XPCS Operations with ALCF Computing Resources

Technical Achievement

A team comprising staff at the APS, the Argonne Leadership Computing Facility (ALCF), and the Data Science & Learning (DSL) division have successfully demonstrated the first use during APS beam time of the new ALCF Polaris testbed

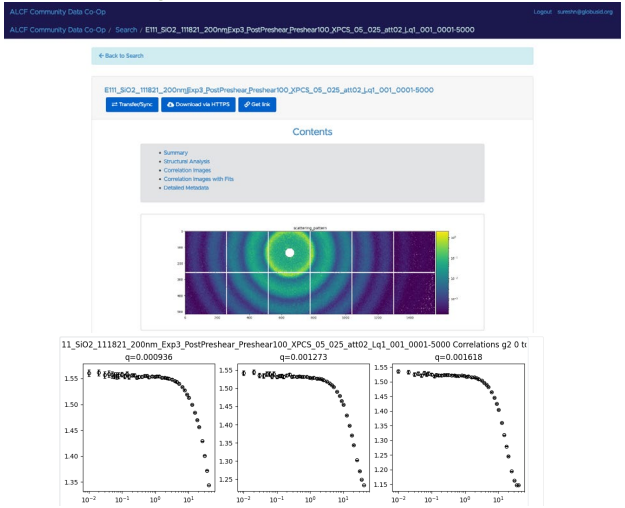
Significance and Impact

This work lays the path to utilization of the new Polaris supercomputer and the soon to be delivered Aurora supercomputer, for routine use at APS instruments for facile real-time and post-experiment data processing and analysis by both APS staff and APS users (on-site and remote)

Research Details

- APS-developed high-performance computing software, XPCS-Eigen, is deployed on the Polaris testbed for data processing
- The APS Data Management System is integrated with Globus Gladier/FuncX workflow tools to provide a single end-to-end data pipeline
- A convenient web-based data portal enables staff and users (on-site and remote) to view data as it's acquired and processed in near real-time

Artist rendering of the new ALCF Polaris supercomputer.



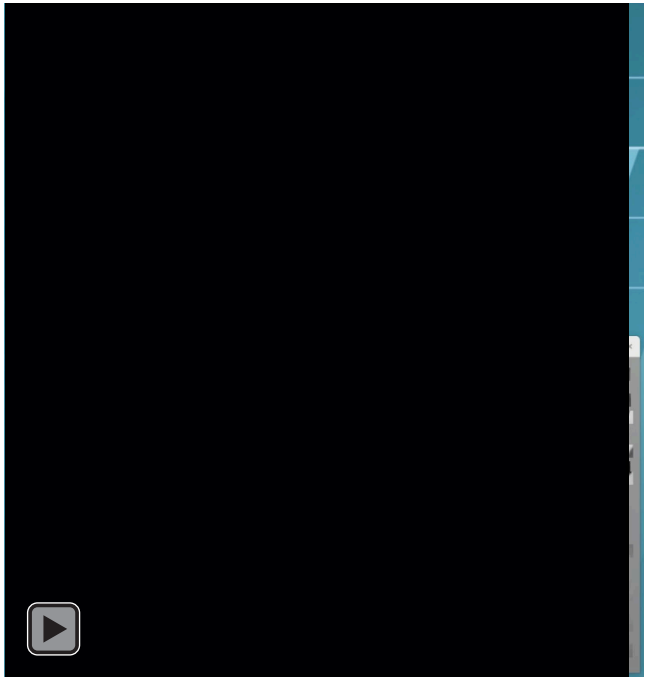
Web-based data portal accessible to on-site and remote users showing processed XPCS data from APS 8-ID beamline.

XSD: Suresh Narayanan, Hannah Parraga, Faisal Khan, Miaoqi Chu, Sinisa Veseli, John Hammonds, Nicholas Schwarz; ALCF: Ryan Chard, Nickolaus Saint, Rafael Vescovi, Ben Blaiszik, Ian Foster

AI@EDGE ENABLES REAL-TIME PTYCHOGRAPHY

Train AI @ ALCF, deploy AI @ beamline

Work led by Tao Zhou, Anakha Babu and Saugat Kandel with contributions from Yi Jiang, Yudong Yao, Sinisa Veseli, Tekin Bicer, Zhengchun Liu, Michael Wojcik, Martin Holt, Antonino Miceli and Mathew Cherukara



- Real-time imaging: >100× faster than phase retrieval
  - Demonstrated live inference at 100 Hz on 512×512-pixel detector images
- Lower-dose imaging : 25× less data than phase retrieval
- Future work: other techniques, closed-loop experimental steering