Message from the Editors

Welcome to the third issue of the **Division of Computational Physics (DCOMP)** Newsletter. In this issue, we introduce our new executive committee members, summarize DCOMP-related activities to attend at GPS 2026 and begin preparing for GPS 2027. We are thrilled to introduce six new fellows and the newly established Charlotte Froese-Fischer Mid-Career Award.

Thank you for reading — we are excited to continue sharing the accomplishments and activities of our vibrant community.

Sincerely,
Sahar Sharifzadeh and Neepa Maitra
on behalf of the DCOMP Executive Committee

DCOMP Executive Committee Welcomes New Members!

As a result of our recent elections, Prof. Helvi Witek (University of Illinois, Urbana-Champaign, UIUC) will come on board as Vice Chair, joining Chair-Elect Sahar Sharifzadeh (Boston University), Chair André Schleife (UIUC), and Past Chair Koblar Alan Jackson (Central Michigan University). We are grateful for the work of Eva Zurek (University of Buffalo) who served as Chair and Past Chair in the past two years, and now will rotate out of the chair line.

Two new members-at-large, John Lyons (U.S. Naval Research Laboratory, NRL) and John Pask (Lawrence Livermore National Laboratory), will join Michael Zingale (Stony Brook University, SUNY), Aidan P Thompson (Sandia National Laboratories), Neepa T Maitra (Rutgers University - Newark), Volker Blum (Duke University), and student member-at-large Francesco Belli (SUNY-Buffalo). Two current members Michelle Johannes (U.S. NRL) and Roxana Margine (Binghamton University) will rotate out of the at-large committee.

Secretary/Treasurer Marivi Fernandez (Stony Brook University) and Councilor Amy Y Liu (Georgetown University) will remain on the committee for the next year.

Prof. Witek is an internationally recognized expert in gravitation, numerical relativity, and gravitational waves. Numerical relativity refers to the development and use of High-Performance Computing cyber-infrastructures to numerically model the coalescence of black holes and neutron stars. She is the co-PI of the Einstein Toolkit, an open-source software infrastructure for computational

Helvi Witek, Vice Chair

astrophysics with 460+ registered members worldwide. She was a co-chair of the LISA Waveform Working Group from 2018 – 2024. LISA stands for Laser Interferometer Space Antenna, a space-based gravitational wave detector mission adopted by ESA and NASA.

John Lyons is a physical scientist in the Theory of Advanced Materials Section at the US Naval Research Laboratory (NRL) in Washington, DC. He joined NRL in 2016 after a post-doctoral fellowship at the Center for Functional Nanomaterials at Brookhaven National Laboratory, before which he earned his PhD in Materials at the University of California, Santa Barbara in 2012, and his BS in Materials Science and Engineering at the University of Wisconsin, Madison in 2008. At NRL, John uses first-principles density functional theory calculations to investigate ultrawide-bandgap semiconductors and novel electronic materials. He is also one of our newly elected 2025 DCOMP fellows.

John Lyons, Member-at-large

John Pask is a Senior Staff Physicist at the Lawrence Livermore National Laboratory (LLNL). Before joining LLNL, he taught mathematics, physics, and reactor dynamics at the United States Naval Nuclear Power School in the 1990s. He received a Ph.D. in physics from the University of California at Davis in 1999, after which he worked as a National Research Council Postdoctoral Associate at the United States Naval Research Laboratory (NRL) and as a member of postdoctoral staff at LLNL before joining LLNL as a Staff Physicist in 2004. He has worked in the field of electronic structure methods development and applications for the better part of the last three decades. He is a pioneer in the development of real-space methods for large-scale calculations, with applications ranging from catalysis and defect formation at/near ambient conditions to equation of state and transport properties at extreme conditions of temperature and pressure.
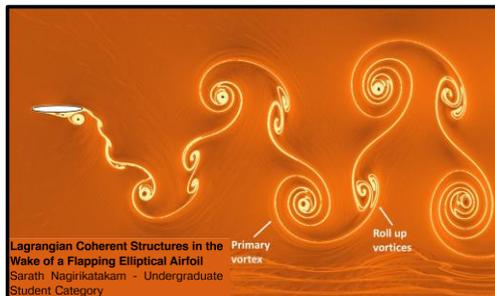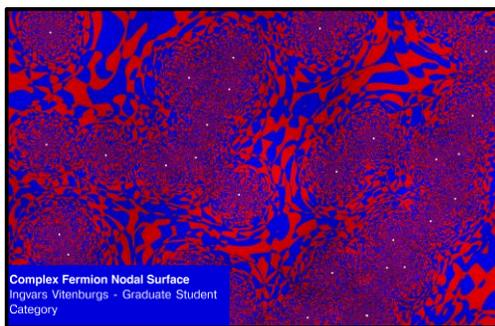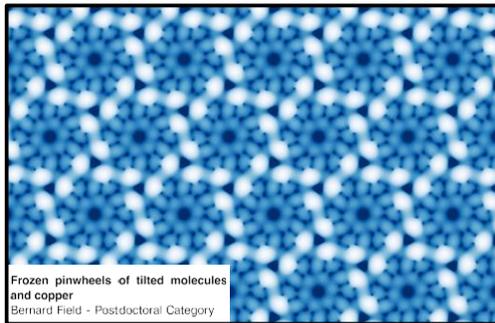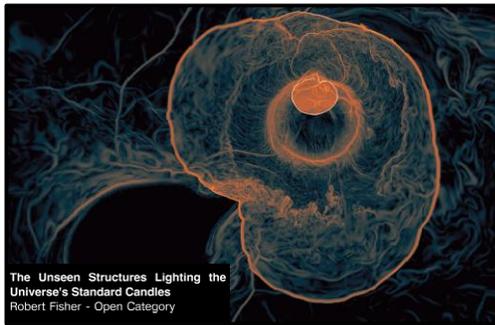
John Pask, Member-at-large

Charlotte Froese-Fischer Mid-Career Award: Get your nominations ready!

DCOMP has established an award to recognize outstanding contributions by a mid-career scientist in the broad field of computational physics, including, for example, condensed matter, non-equilibrium dynamics in molecules and materials, astrophysics, biological modeling, statistical physics, high-performance computing, and artificial intelligence. This award is named in honor of Charlotte Froese Fischer, an early pioneer in computational physics. Keep an eye out for a call for nominations coming soon!

DCOMP at the Global Physics Summit 2026

We look forward to seeing you in Denver March 15-20, 2026!

DCOMP is sponsoring a number of Focused Topic and Invited sessions that span many topics within computational physics with 21 travel grants awarded to students and postdocs to enable their attendance this year. Make sure to visit the DCOMP Table and check out our image competition winners shown in the Figure below. All of our submissions can be found at: $https://engage.aps.org$.

The Unseen Structures Lighting the Universe's Standard Candles
Robert Fisher - Open Category

Frozen pinwheels of tilted molecules and copper
Bernard Field - Postdoctoral Category

Complex Fermion Nodal Surface
Ingvars Vitenburgs - Graduate Student Category

Lagrangian Coherent Structures in the Wake of a Flapping Elliptical Airfoil
Sarath Nagirikatakam - Undergraduate Student Category
Primary vortex
Roll up vortices

We would like to highlight the following DCOMP-sponsored events:

- DCOMP is co-sponsoring squishy science again this year, together with DSOFT. The event will take place at the Denver Museum of Nature and Science. Join us on Sunday March 15 for hands-on activities about physics, including the physics of slime, sand, and cotton candy.

- The DCOMP business meeting will be held on Wednesday, March 18, at 6:30 PM. (Location Convention Center, Meeting Room 601)

Refreshments will be provided!

- The DCOMP Award Session at the GPS will also be held on Wednesday, 12 pm - 3 pm. The location will be Convention Center, Bluebird 1A. The session starts with Metropolis Dissertation Award winner Benjamin Xu Shi (Flatiron Institute) followed by the Rahman Prize recipient Stefano Baroni (Scuola Internazionale Superiore di Studi Avanzati). These talks will be followed by three speakers who will speak on the topic of research software engineering (RSE): Gabriele Bozzola (AWS Center for Quantum Computing); Calvin Li (FUM); Geoffrey Lovelace (California State University, Fullerton).

- Here are our Focus Topic Sessions at GPS 2026:

    - Electron-Phonon, Exciton-Phonon, and Phonon-Phonon Interactions
    - First-Principles Modeling of Excited-State Phenomena in Materials
    - Machine Learning for Atomistic Simulation
    - Precision Many-Body Physics
    - First-Principles Simulations of Electron Transport and Dynamics
    - Computational Methods for Statistical Mechanics: Advances and Applications
    - Recent Applications and Developments in Quantum Embedding
    - Machine Learning Potentials, Foundational Models, Molecular Dynamics and Monte Carlo for Materials Research
    - Interfacial Charge, Spin, and Chemical Dynamics in Energy and Quantum Materials
    - Extreme-Scale Computational Science Discovery in Fluid Dynamics and Related Disciplines
    - Computational Design, Understanding, and Discovery of Novel Materials
    - Advances in Computational Physics for Fusion Applications
    - Theory and Simulation for Non-Equilibrium Quantum Physics of Materials
    - Advances in Simulation and Modeling of Liquid Solutions and Solid–Liquid Interfaces
    - Modern Atomistic Modeling of Disordered Materials
    - Density Functional Theory at the Intersection of Traditional Electronic Structure Theory and AI/ML
    - Dopants and Defects in Semiconductors
    - Fe-Based Superconductors: New Tuning Knobs
    - 2D Materials: Frontiers of Van der Waals Assembly and Moiré Materials
    - Multiferroics, Magnetoelectrics, Spin-Electric Coupling, and Ferroelectrics

   – Matter at Extreme Conditions

   – Quantum-Classical Hybrid Learning and Quantum Simulations

   – Machine Learning Force Fields and Surrogate Models for Atomistic Simulations

• Here are our Invited Sessions at GPS 2026, this includes DCOMP sponsored, co-sponsored, and cross-cutting (between March and April meeting) invited sessions:

   – Advances in the Theory of Altermagnetism

   – Electron dynamics and spin transport in molecular electronics devices

   – Reliable Effective Models for Correlated Electrons

   – Chirality-Induced Spin Selectivity: Theory and Computation

   – Computational Physics and Machine Learning for Optimizing Energy Conversion and Flow

   – First-principles modeling of nonlinear interactions in materials

   – Monte Carlo Simulations in Condensed Matter and Nuclear Systems I and II

   – AI in Different Aspects of Gravitational Waves

   – Scaling Big Codes to Bigger Computing

• In addition, this short course was organized by DCOMP members:

   – "Electron-phonon physics from first principles" organized by Roxana Margine, Feliciano Giustino, and Sabyasachi Tiwari

GPS 2027: Accepting Proposals for Focus Topic and Invited Sessions Hosted by DCOMP

Please reach out to chair-elect Sahar Sharifzadeh (*sshari f z@bu.edu*) if you are interested in proposing Focus Topic and Invited Sessions for the 2027 Global Physics Summit, that will be held April 11-16 in Atlanta, Georgia.

Meet the New DCOMP Fellows

Congratulations to the six new fellows elected by DCOMP this year!

For pioneering work in high-throughput computational materials design and discovery, especially in the field of quantum and opto-electronic materials.

Geoffroy Hautier

For pioneering the application of artificial intelligence to materials discovery, including interpretable and generative models for quantum materials, and for developing widely used software tools that have advanced computational methods in energy, electronics, and superconductivity.

Richard G. Hennig

For pioneering contributions to the use of atomistic simulation to study the equilibrium and nonequilibrium properties of interfaces and significant advances in the development of algorithms for molecular-dynamics simulation.

Brian Bostian Laird

For fundamental contributions to the understanding and design of wide-bandgap semiconductors using first-principles methods, including strategies for semiconductor doping and for understanding and controlling exciton fine structure.
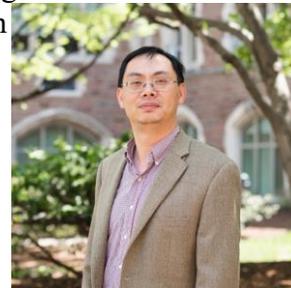
John L. Lyons

For contributions to computational discovery and design of materials via the development of methods and codes for structure and property prediction of molecular crystals, as well as organic, inorganic, and hybrid interfaces.

Noa Marom

For developing and utilizing ab initio simulations to understand many-electron interactions at the nanoscale and predicting emerging electronic, optical, and magnetic properties in reduced-dimensional structures.

Li Yang