

# CSP NEWS



## The University of Georgia - Center for Simulational Physics (CSP)

### CSP Members

#### David P. Landau, CSP Director

**CSP Faculty:** Michael Bachmann, Michael R. Geller, Cassandra Hall, David P. Landau, Steven P. Lewis, H.-Bernd Schüttler (Assoc. Dir.), Robin L. Shelton, and Phillip C. Stancil

**Adjunct:** Kurt Binder, Robert Buenker, Wolfhard Janke, Brendan McLaughlin, Joao Plascak, Dennis Rapaport, Robert Swendsen, Shan-Ho Tsai, and Thomas Wuest

**Research Staff/Visitors:** Benhui Yang,

**Graduate Students:** Dilimulati Aierken, Mona Asadi Namin, Yifan Dai, Garrett Floyd, Kellan Gibson, Eric Goetz, Steven Hancock, Zizhe Hu, Anastashia Jebraeilli, Nima Karimitari, Maninder Kaur, Darin Mihalik, Matthew Murray, James Sargent, Kedkanok Sitarachu, Eric Suter, Zahra Taghadomi, Jason Terry, Chen Wang, Ruihan Wang, Sydney Whilden, Matthew Wilson, Aojie Xue, and Susannah Zhang

**Undergraduate Students:** Alex Bergeron, Nabuchi Budendwa, Robert Bull, Joshua Courtney, Anson Dao, Ana Jabraeilli, Jordon Kale, Nick Kruegler, Laney Norton, Rinisha Ramprakash, Catherine Schilling, Remie Tule, and M. Elliott Williams

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**Many thanks to all who have given  
to the CSP fund!**



### Message from the Director

During the last half of 2021 the CSP continued to face challenges due to the pandemic but some improvement was evident. Since UGA had made vaccinations available, without cost, for all students and faculty, many CSP members were beginning to return to their workspaces. But the wearing of masks and social distancing was clearly evident. The CSP lunch seminar remained virtual, and we had a rich variety of talks with both speakers and attendees from the international community. Planning has begun for next year's 35th Annual CSP Workshop which will again be held in a purely virtual format because of the remaining danger from Covid-19. We also anticipate holding the postponed Quantum Computing Workshop and U.S.-China Bilateral Symposium next spring. Final decisions will depend upon the status of the pandemic. Lastly, I would like to thank all of you who have donated to the CSP Alumni Foundation Fund. Best wishes to everyone for a happy and HEALTHY 2022.

### CSP Happenings

The American Astronomical Society Summer Conference, which includes the meeting of the Laboratory Astrophysics Division, was held virtually in June 2021. As LAD Chair **Prof. Phillip Stancil** co-organized the meeting, chaired a plenary and invited talk session, and presented a virtual poster "Non-LTE rovibrational analysis of carbon sulfide in photodissociation regions"

On Nov.28 **Prof. David P. Landau** presented an Invited Talk at **The International Conference on Multidisciplinary Approaches in Science, ICMAS-2021** in Colombo, Sri Lanka. The title of his talk was "Exploring Complex Free Energy Landscapes with Innovative Monte Carlo Simulations".

**Prof. Cassandra Hall** has been elected a Fellow of the Royal Astronomical Society. She also presented an Invited talk at the APS SESAPS meeting Nov. 18-20.

On Nov. 6 **Prof. Robin Shelton**, Eric Goetz, Chen Wang, and Sydney Whilden presented their simulational work at the Georgia Regional Astronomers Meeting at Georgia Tech, demonstrating that high velocity clouds and intergalactic clouds are 6 to 10 times heavier than previously thought. This ramifications for the evolution of the Milky Way is that high velocity clouds are suppling it with far more material for star formation than was expected.

## *In The News*

UGA undergraduate Sean McIlvane; graduate students Darin Mihalik, Zahra Taghadomi, and Ruihan Wang; and research scientist Benhui Yang gave virtual posters at the Summer American Astronomical Society meeting held virtually in June.

On Sept. 24 Prof. David P. Landau presented a seminar at the Universität Mainz, Germany: "Effects of Lattice Constraints on Folding in the Semi-Flexible HoP Protein Model: A Wang-Landau Study".

From Oct. 14 - 22 Prof. David P. Landau participated in virtual meetings of the Council and Commission Chairs of the International Union of Pure and Applied Physics (IUPAP) and the IUPAP General Assembly. He has been Chair of the C20 Commission on Computational Physics since 2018 and is also Chair-Elect of the U.S. Liaison Committee between the U.S. National Academy of Sciences and IUPAP.

Prof. Cassandra Hall has received two grants of ALMA telescope time.

During the XXXII IUPAP International Meeting on Computational Physics CCP2021, Matthew Wilson and David Landau presented a paper "Comparison of Benchmark HP Lattice Proteins on Simple-Cubic and Face-Centered Cubic Lattices Using Replica-Exchange Wang-Landau Sampling", and Alfred Farris and David Landau presented a paper "Replica exchange Wang-Landau sampling of long HP lattice protein sequences."

In November Prof. David P. Landau participated in a meeting of the Rektor's Academic Advisory Council (AAC) of Heidelberg University in Germany. The AAC advises the Rektor on strategic initiatives for the university. This small panel of international experts is chosen from a broad range of disciplines.

Jason Terry from Prof Hall's group presented a talk at the 88th Annual Meeting of the American Physical Society Southeastern Section

A former undergraduate in Prof. Phillip Stancil's group, Patrick Mullen, is now a postdoctoral fellow at the Institute for Advanced Study at Princeton. He obtained a BS in Physics at UGA in 2015 and a PhD at the U. of Illinois.

As Chair of the IUPAP C20 Commission on Computational Physics, **Prof. David P. Landau** opened the XXXII IUPAP Conference on Computational Physics CCP2021. During CCP2021 Prof. Landau also awarded the 2020 and 2021 Young Scientist Prizes and chaired a (Zoom) meeting of the C20 Commission.

**Prof Cassandra Hall's** research was featured in a News Release from the National Radio Astronomy

Observatory <https://public.nrao.edu/news/chaotic-young-star-reveals-planet-formation/>, and also in the Sky and Telescope magazine <https://skyandtelescope.org/astronomy-news/gravitationally-unstable-disk-may-collapse-to-form-planets/>

**Dr. Steven Lewis** and Eric Suter submitted a paper to Applied Physics on transition-metal dopant trends in the electronic structure of KNbO<sub>3</sub>. Dr. Lewis and Nima Karimitari submitted a paper to Surface Science on the structure and vibrations of c(4x2) PF<sub>3</sub> on Cu(001).

**Prof. Bernd Schüttler**, in collaboration with students and faculty colleagues from the Department of Genetics and the IOB is developing novel modeling tools in functional genomics, based on computational methods derived from statistical physics. One specific application is the identification of sets of multiple genes which together produce quantitative traits (QTs) in living organisms.

## Student Awards

UGA undergraduate student, Nick Kruegler, has a CURO Research Award (formerly CURO Research Assistantship) during fall semester.

Elijah Courtney, from Dr. Stancil's group, received the Department's Charles H Wheatley Award for Outstanding Senior Physics student. He is now a Physics PhD student at Stanford U.

Laney Norton received the Department's Linville L. Hendren Memorial Scholarship. She is currently a senior astrophysics major studying molecular emission from circumstellar envelopes.

## Student Degrees

### Matthew Wilson, PhD Physics

In Fall 2021, Matthew Wilson successfully defended his PhD thesis on Replica-exchange Wang-Landau Simulation of face-centered cubic lattice models for protein folding and peptide aggregation, under the direction of Prof. David Landau. He will work as a postdoctoral research associate at Los Alamos National Lab starting in Spring 2022.

