

Annual Review of HEDP-Theory Group Performance for 2023

S. X. Hu, Valentin Karasev, Shuai Zhang, Nathaniel Shaffer, Katie Hilleke, Adrien Pineau, Deyan Mihaylov, Brennan Arnold, John Cappelletti, Justin D'Souza, Dylan Durkee, Maitrayee Ghosh, Rati Goshadze, Josh Hinz, Katarina Nichols, Ioannis Pagiazitis, Annie Maloney, Kaan Aytekin, Courtney Palmeri, Cody Reeth, Marcos Ibanez

HED-t @ 2023



HED-t Members
(as of 12/2023)

7 Scientists

9 PhD Students

5 Undergrads

(a new group photo needed)

HEDP-Theory Group Meeting

on 12/15/2023

Mission & Vision Statements are drafted for HEDP-Theory Group

Our Mission

- Developing accurate *first-principles* physics models of HED material properties (EOS, Opacity, Transport), to enable reliable LDD fusion target designs and simulations of ICF experiments at LLE;
- Exploring how matter behaves under extreme conditions, to discover new HED physics and chemistry phenomena;
- Educating/Preparing PhD and undergraduate students to become next-generation stewards for NNSA's SSP and science missions.

Our Vision

- Innovating new theoretical and computational capabilities is key to advance our understanding of HED physics and chemistry;
- Bridging the microscale HED physics to meso-/macro-scale observations, in close collaboration with experimentalists, is critical to make new discoveries;
- Embracing advancements in Machine Learning, Artificial Intelligence, and Quantum Computing is important to stimulate scientists and students for future success

Four research thrusts are currently undertaken by scientists and graduate/undergraduate students in the HEDP-Theory Group at LLE

HEDP Research Thrust Areas (overseen by Dr. Suxing Hu)

Equation-of-State (EOS) (led by Dr. Valentin Karasiev)

- Developing advanced temperature-dependent exchange-correlation functionals to improve DFT accuracy
- Developing the finite-element based DFT code *MELIORA* to tackle challenging conditions (shock release)
- Using *Machine Learning* to ensure thermodynamic consistency of EOS

Opacity (led by Dr. Nathaniel Shaffer)

- Developing next-generation plasma atomic code that combine DFT-inferred plasma screening with detailed atomic structure calculations
- Providing dense-plasma atomic data for interpreting x-ray spectroscopy experiments on OMEGA
- Supporting radiation transport work in LLE rad-hydro codes

Dynamic/Kinetic Modeling (led by Dr. Shuai Zhang)

- Large-scale classical molecular-dynamics modeling of shock release
- Kinetics of phase transition of materials under extreme HED conditions
- Utilizing Machine-Learning and AI to derive reliable potentials for reactive HED materials

Future Capabilities for HED Physics (led by Dr. Suxing Hu)

- Developing finite-element mixed-DFT and TD-DFT code "MELIORA"
- Quantum computing for HED physics
- Developing in-house modeling capability to connect microscale to meso-/macro-scale

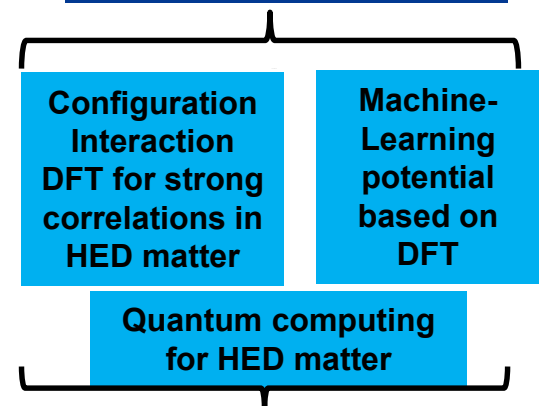
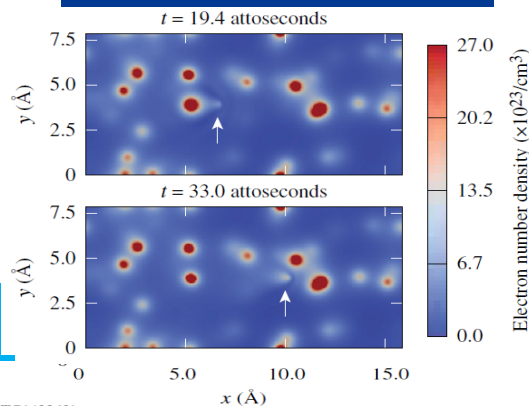
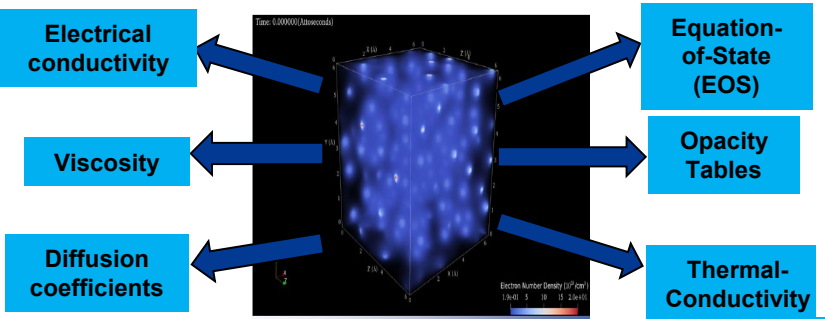
Our strategic plan: Significant advances in improving and developing new *first-principles* computational methods are expected to shift the paradigm for HED physics research at LLE in next five to ten years



Quantum Molecular-Dynamics* (QMD) based on today's DFT

TD-DFT (state-of-the-art for HEDP)

The future of *first-principles* HED Physics



Static/Transport/Optical properties of HED matter @ micro-scale (< ~1000 atoms)

Dynamic properties of HED matter @ micro-scale (< ~50,000 atoms)

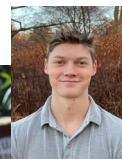
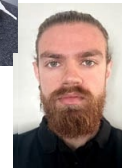
Connecting micro-scale to meso-/macro-scale (~million-to-billion atoms)

*S. X. Hu, V. V. Karasiev, V. Recoules, P. M. Nilson, N. Brouwer, M. Torrent, *Nature Communications* **11**, 1989 (2020).
 V. V. Karasiev, J. Hinz, S. X. Hu, S. B. Trickey, *Nature* **600**, E12 (2021).
 S. X. Hu, D. T. Bishel, D. A. Chin, P. M. Nilson, V. V. Karasiev et al., *Nature Communications* **13**, 6780 (2022).

What's new in 2023?

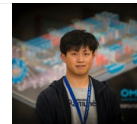
- **Eight (8) new members have joined our group in 2023:**

- **Katie Hilleke (Assistant Scientist):** from University of Buffalo (bringing high-pressure chemistry expert to our group)
- **Ioannis Pagiazitis (first-year):** PhD student from UoR's ME department (advised by S. X. Hu; working on Quantum Computing for HEDP)
- **Kaan Aytekin:** Undergrad from ME, working on laser absorption (advised by N. Shaffer)
- **Courtney Palmeri:** Undergrad from CE, working on HED materials (advised by S. Zhang)
- **Annie Maloney:** Undergrad from PAS, working on radiation levitation (advised by S. X. Hu)
- **Cody Reeth:** Undergrad from CS+PAS, working on MELIORA code (advised by S. X. Hu)
- **Marcos Ibanez:** Undergrad from CS+Math, working on MELIORA code (advised by S. X. Hu)
- **Cian Baldwin:** Summer intern from Yale University, working hybrid kinetic-fluid modeling of laser plasmas (advised by N. Shaffer)



Education Achievement/News in 2023

- [Maitrayee Ghosh](#), from Department of Chemistry and advised by Dr. S. Zhang, has successfully defended her PhD thesis on November 8th, 2023. Dr. Ghosh is heading to SLAC/Stanford University for her postdoc fellowship. Congrats to Maitrayee!
- Two Horton Fellows (graduate students) successfully passed their PhD qualify exam at Department of Physics & Astronomy:
 - [Rati Goshadze](#) (advised by Dr. V. Karasiev)
 - [Katarina Nichols](#) (advised by Dr. S. X. Hu)
- [John Cappelletti](#) (Horton Fellow), from ME and advised by Dr. S. X. Hu, has won “Outstanding Poster” award in LANL’s summer school of Parallel Computing.
- [Lianming Hu](#), an undergrad from ME and advised by Dr. S. Zhang, got into the graduate program at MIT.
- [Dr. S. X. Hu](#) was jointly appointed as *Professor of Physics (Research)* and *Professor of Mechanical Engineering (Research)* at University of Rochester.



We continue contributing to advances in HED sciences, serving the HED physics community, and enhancing our DEI efforts



- Published/Submitted **19 first-authored papers** in peer-reviewed scientific journals, including **9 papers are from PhD students** (*a sign of recovery from the pandemic*)!
- Contributed to **11 co-authored papers** published in peer-reviewed scientific journals
- HEDP-Theory Group members **gave Plenary/Invited Talks and Colloquium** at conferences & universities (contributing to LLE's visibility)
- Collaborations with **LLE Groups of HEDx/IM/LPI/Optical-Materials, as well as National Labs and other Universities** have been continuously strengthened in 2023
- HEDP-Theory Group members continued to **serve the scientific community** by organizing workshops, severing PhD defense committees, and reviewing for grants and journals
- **DEI efforts**: Group members attended DEI seminars; PhD candidate K. Nichols chaired LLE-WISE Group and organized DEI/Career seminars; K. Nichols & S. X. Hu gave lectures to LLE's BEST high-school program

Nineteen (19) first-authored papers have been published (or submitted) by HED-t members (underlined) in 2023



1. M. Ghosh** , S. Zhang, L. Hu, S. X. Hu, “*Cooperative diffusion in body-centered cubic iron at Earth and super- Earth inner-core conditions*”, *J. Phys.: Condens. Matter* **35**, 154002 (2023).
2. R. M. N. Goshadze** , V.V. Karasiev , D. I. Mihaylov , S. X. Hu, “*Shock-induced metallization of polystyrene along the principal Hugoniot investigated by advanced thermal density functionals*”, *Phys. Rev. B* **107**, 155116 (2023).
3. J.P. Hinz** , V.V. Karasiev, S. X. Hu , D.I. Mihaylov, “*Development of a machine-learning-based ionic-force correction model for quantum molecular dynamic simulations of warm dense matter*”, *Phys. Rev. Materials* **7**, 083801 (2023).
4. K.A. Nichols** , S. X. Hu, A. J. White, V. N. Goncharov, D. I. Mihaylov, L. A. Collins, N. R. Shaffer, V. V. Karasiev, “*Time-dependent density-functional-theory calculations of the nonlocal electron stopping range for inertial confinement fusion applications*”, *Phys. Rev. E* **108**, 035206 (2023).
5. S. Zhang, R. Paul** , S. X. Hu, M. A. Morales, “*Toward an accurate equation of state and B1-B2 phase boundary for magnesium oxide to TPa pressures and eV temperatures*”, *Phys. Rev. B* **107**, 224109 (2023).
6. N. R. Shaffer, A. V. Maximov, and V. N. Goncharov, “*Thermal conductivity of a laser plasma*”, *Phys. Rev. E* **108**, 045205 (2023).
7. N. R. Shaffer, M. Sherlock, A. V. Maximov, and V. N. Goncharov, “*An extended Vlasov-Fokker-Planck approach for kinetic simulations of laser plasmas*”, *Phys. Plasmas* **30**, 043906 (2023).
8. D.I. Mihaylov, S.X. Hu, and V.V. Karasiev, “*Dragon: A multi-GPU orbital-free density functional theory molecular dynamics simulation package for modeling of warm dense matter*”, *Comput. Phys. Commun.* **294**, 108931 (2024).
9. S. X. Hu, ...K. A. Nichols** , R. M. N. Goshadze** , M. Ghosh** , J. Hinz** , V. V. Karasiev, S. Zhang, N. R. Shaffer, D. I. Mihaylov, J. Cappelletti** , ...C. Deeney, “*Laser-direct-drive fusion target design with a high- gradient-density pusher shell*”, *Phys. Rev. E* **108**, 035209 (2023).

Nineteen (19) first-authored papers have been published (or submitted) by HED-t members (underlined) in 2023 [Cont.]



10. K. P. Hilleke, R. Franco, P. Pertierra, M. A. Salvado, E. Zurek, J. M. Recio, “Preference for a pressure-induced 3D structure after 1T-HfSe₂”, *Mater. Today Phys.* **36**, 101152 (2023).
11. K. P. Hilleke, X. Wang, D. Luo, N. Geng, B. Wang, F. Belli, E. Zurek, “Structure, stability, and superconductivity of N-doped lutetium hydrides at kbar pressures”, *Phys. Rev. B* **108**, 014511 (2023).
12. V. V. Karasiev, J. Hinz** , and R.M.N. Goshadze** , “Framework for Laplacian-level noninteracting free-energy density functionals”, *Phys. Rev. Lett.* (submitted).
13. V. V. Karasiev, D.I. Mihaylov, S. Zhang, J.P. Hinz, R.M.N. Goshadze, and S.X. Hu, “Tunable noninteracting free-energy density functionals for high-energy-density applications”, *Phys. Plasmas* (submitted).
14. D. Durkee** and S. X. Hu, “Breaking up CO₂ through pressure-induced redox reaction with rhenium”, *Phys. Rev. B* (submitted).
15. M. Ghosh** , S. Zhang, S. X. Hu, “Direct observation of diamond co-existence with hydrocarbon fluids using large-scale density-functional theory simulations in ice giant interior conditions”, *Phys. Rev. B* (submitted).
16. J. Hinz** , D. Yu, ..., D. I. Mihaylov, V. V. Karasiev, S. X. Hu, “The development of thermodynamically-consistent and physics-informed equation-of-state model through machine learning”, *APL: Machine Learning* (submitted).
17. A. Pineau, H. Trollvik, S. Olsen, Y. Eilertsen, and I. Mann, “Simulations of the collection of mesospheric dust particles with rocket instrument”, *Atmospheric Measurement Techniques* (submitted).
18. J. D'Souza** , ..., S. Zhang. “Temperature and Density Dependent Pair Potential for Deuterium Under Shock”, *AIP Conf. Proc.* (submitted).
19. M. Ghosh** , S. X. Hu, E. Blackman, S. Zhang, “Melting and metallization of Al₂O₃ at extreme conditions”, *Phys. Rev. B* (submitted).

HEDP-Theory Group members (underlined) contributed to eleven (11) co-authored papers published in 2023

1. D. Turnbull, ..., N. R. Shaffer, *et al.*, *Phys. Rev. Lett.* **130**, 145103 (2023).
2. C. E. Starrett and N. R. Shaffer, *Phys. Rev. E* **106**, 025204 (2023).
3. I. V. Igumenshchev, ..., N. R. Shaffer, *et al.*, *Phys. Rev. Lett.* **131**, 015102 (2023).
4. W. A. Angermeier, B. S. Scheiner, N. R. Shaffer, and T. G. White, *Phil. Tran. R. Soc. A* **381**, 20230034 (2023).
5. R.W. Paddock, ... R.M.N. Goshadze, V.V. Karasiev, and S.X. Hu, *Phys. Rev. E* **107**, 025206 (2023).
6. S Jiang, ..., S. X. Hu, G. W. Collins, Y. Ping, *Communications Physics* **6**, 98 (2023).
7. A Lees, ..., S. X. Hu, ...CA Thomas, *Phys. Plasmas* **30**, 012709 (2023).
8. V. Gopaldaswamy, ..., S. X. Hu, ..., C. Deeney, *Nat. Phys.* (in press).
9. C. A. Williams, ..., S. X. Hu, ..., E. M. Campbell, *Nat. Phys.* (in press).
10. K. R. P. Kafka, S. X. Hu, H. Huang, V. N. Goncharov, S. G. Demos, *Phys. Rev. Res.* (in press).
11. G. Tabak, ..., S. Zhang, S. X. Hu, ..., G. W. Collins, *Phys. Rev. B* (in press).

HEDP-Theory Group members gave invited presentations to conferences/workshops in 2023



- Katarina Nichols** , “Time-Dependent Density-Functional-Theory Studies of Nonlocal Electron Stopping Range in ICF Plasmas”, [The 65th Annual Meeting of the APS Division of Plasma Physics, Denver, CO \(invited\)](#).
- Katarina Nichols** , “*TD-DFT Calculations of the Nonlocal Electron Stopping Range for Inertial Confinement Fusion Applications*”, [The 2nd Workshop on Charged-Particle Transport in HED Plasmas , Livermore, CA \(invited\)](#).
- Shuai Zhang , “*Setting Constraints on the Equation of State and Phase Behaviors of Planetary Materials from First Principles*”, [AGU Fall Meeting, San Francisco, CA \(Invited\)](#)
- Shuai Zhang , “*Turning up the Heat on High Energy Density Materials in Silico — Case Studies*”, [Joint CDAC/CMEC Webinar, University of Illinois, Chicago, IL \(Invited\)](#)
- Nathaniel Shaffer , “*Thermal conductivity of a laser plasma*”, [LLNL High Energy Density Science Seminar, Livermore, CA \(invited\)](#).
- Nathaniel Shaffer , “*Electron transport from mean-force quantum Landau-Fokker-Planck theory*”, [The 2nd Workshop on Charged-Particle Transport in HED Plasmas, Livermore, CA \(invited\)](#).
- Nathaniel Shaffer , “*Recent progress in transport theory for high-energy-density plasmas*”, [International Conference on High Energy Density Science, Yokohama, Japan \(invited\)](#).
- Valentin Karasiev , “*Predicting material properties in the warm-dense matter regime with use of thermal exchange correlation density functionals*”, [The 2nd Workshop on Charged-Particle Transport in HED Plasmas \(invited\)](#).
- S. X. Hu , “*Probing Extreme Atomic Physics in Super-dense Plasmas*”, [International Conference on Atomic Processes in Plasmas, Vienna, Austria \(invited\)](#).
- S. X. Hu , “*Probing Warm-Dense Matter with X-ray Spectroscopy*”, [International Workshop on Warm Dense Matter, Awaji Island, Japan \(invited\)](#).
- S. X. Hu , “*Probing High-Energy-Density Matter with X Rays*”, [Photon Science Seminar, SLAC/Stanford University, CA \(invited\)](#).

External collaborations with National Labs and other Universities are continuously strengthened

- **Collaborations with LANL are actively pursued in the following three fronts:**
 - ❑ With L. A. Collins & A. White on TD-mDFT development for stopping power and non-local electron thermal transport [K. Nichols (Horton Fellow), D. Mihaylov, N. R. Shaffer & S. X. Hu]
 - ❑ With J. Daligaut and D. Saumon on white-dwarf physics (B. Arnold (Horton Fellow) & S. X. Hu)
 - ❑ With C. Starrett on average-atom model and transport in WDM (N. R. Shaffer)
- **Collaborations with LLNL can be further strengthened:**
 - ❑ High-pressure physics of materials (S. Zhang, C. Wu, T. Ogitsu, *et al.*)
 - ❑ VFP simulation of LPI (N. R. Shaffer, M. Sherlock)
- **Collaboration with SNL on dense plasma and atomic physics:**
 - ❑ Studies on dense plasmas (S. X. Hu, P. Nilson, S. Hansen, I. Golovkin, M. Gu, D. Bishel, A. Chin)
 - ❑ Atomic physics in HED physics (N. R. Shaffer, K. Adler, S. Hansen, T. Gomez, C. Starrett)
 - ❑ TD-DFT calculations of stopping power ((S. X. Hu, K. Nichols, A. Kononov, A. D. Baczewski)
- **Collaboration with CEA on DFT codes enhancement** (V. V. Karasiev, D. I. Mihaylov)
- **Collaboration Prism & UNR:**
 - ❑ FAC/Opacity project (N. Shaffer, S. X. Hu, I. Golovkin, M. Gu, R. Mancini)
- **Collaborations with U. Florida (S. Trickey), U. Buffalo (E. Zurek), PPPL (S. Malko & W. Fox), UC Berkeley (R. Jeanloz, B. Militzer), Flatiron (M. Morales), UNR (T.G. White), Imperial College (G. Kagan), UNL (Y. Lu), Uni. of Basel (S. Goedecker), VCU (G. Miloshevsky), U. Michigan (S. Baalrud), and RIT (Q. Yu) are actively initiated/maintained.**

HEDP-Theory Group members have continued engaging and serving the broad HED physics community in 2023



- **V. V. Karasev**: Co-organizer of a CECAM workshop “*Electronic correlation beyond the ground state*”, Lausanne, Switzerland 15-17 May 2024 (pending approval); Reviewed proposals and manuscripts (1 NSF proposal, 2 Phys. Rev. Lett., 1 Phys. Rev. B, 1 J. Chem. Phys., 1 Comp. Cond. Matter, 1 J. Appl. Phys., 1 Int. J. Quantum Chem)
- **S. Zhang**: Reviewed eight manuscripts (3 PRB, 2 PRR, 1 APL, 1 JGR, 1 JPCM).
- **N. Shaffer**: Served on Ph. D. defense committee of U. Nevada – Reno student William Angermeier; Reviewed five manuscripts (1 Nature Communications, 2 Phys. Rev. E, 1 Atoms, 1 Nuclear Fusion).
- **R. M. N. Goshadze** (Horton Fellow): Reviewed two PRB papers.
- **M. Gosh** (Horton Fellow): Reviewed two PRB papers.
- **S. X. Hu**: Co-organizer of the 2nd Workshop on Charged-Particle Transport in HED Plasmas; Guest Editor for upcoming special issue of Physics of Plasmas; Chaired sessions for CMAP Annual Meeting and NSF Review Meeting; External Examiner for Thomas Gawne’s PhD Thesis (viva) [Oxford University]; Reviewed a bunch of manuscripts for scientific journals.
- **In addition, HEDP-Theory Group hosted the visits and virtual/in-person seminars:** Prof. S. Nakamura (UCSB, 2014 Nobel-prize winner), Prof. B. Ziaja (CFEL/Germany), Prof. N. Abdolrahim (ME/UoR), Dr. M. Gu (Prism), Prof. A. Tamm (U. Tartu), Dr. H.-J. Lee (SLAC), Dr. G. Dyer (SLAC), Dr. A. Bergermann (Uni. Rostock)

Summary: Accomplishments & Highlights for 2023



❑ Scientific Achievements:

- HED-t members first-authored a total of 19 papers published in (or submitted to) peer-reviewed scientific journals, of which 9 papers are from graduate students.
- HED-t members contributed to 11 papers published in scientific journals.

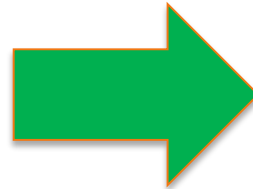
❑ Education Accomplishments:

- **Maitrayee Ghosh**, 2nd PhD student graduated from the HED-t Group, will join SLAC/Stanford University to research on HED materials relevant to planetary science
- **Two PhD students (Horton Fellows)** passed their Qualify Exam at PAS
- **Six undergraduate students** joined in our HEDP-Theory Group in 2023 (starting to *expend our mission in education*)

❑ Highlights for Programmatic Tasks (contribution to LLE experiments):

- **Laser imprint mitigation with foam targets** (*S. X. Hu working with J. Peebles on both planar and cone-in-shell target experiments on OMEGA/EP*)
- **Laser imprint dependence on wavelength** (*A. Pineau working with L. Ceurvorst on planar experiments on OMEGA*)
- **Probing extreme atomic physics with x-ray spectroscopy** (*S. X. Hu, V. V. Valentin working with D. Bishel and P. Nilson on spherical implosion experiments*)
- **Physics of HED materials: Al₂O₃ and SiO₂** (*S. Zhang, M. Ghosh working with T. Suer and M. Marshall on experiments at OMEGA and NIF*)
- **Inverse-Bremsstrahlung laser absorption** (*N. Shaffer working with D. Turnbull on OMEGA experiments*)

Themes @ 2023: “Restarting & Recharging”



Happy Holidays to everyone!!