

Year-End Review of HEDP-Theory Group Performance in 2020



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HEDP-Theory Group Meeting

on 12/17/2020

Despite of the difficulty of Covid-19 pandemic, our HEDP-Theory Group (4 Scientists + 4 PhD-Students) has accomplished a lot in 2020!



- **Successfully completed two important milestones** for our programmatic tasks, with **several accomplishments highlighted** in LLE's Report to NNSA/DOE
- **Published 8 first-authored articles** (including 1 *Nature Commun.*, 1 *PRL*, 2 *PRB*, 1 *PRR*, 1 *PRE*, and 2 others), with **3 first-authored manuscripts** ready for submission
- **Contributed to 15 co-authored papers** in 2020 (including 2 *PRL*, 2 *PRB*, 1 *GRL*,...)
- **Collaborations with HEDx Group, National Labs, CELIA/CEA, and Other Universities** have been further strengthened in 2020
- **One PhD student (Maitrayee) won the IBM-Zerner Graduate Student Award!**
- **Two students (Josh and Reetam) successfully passed their PhD Qualifying Exam!**
- **Group members actively served the broad physics community** by organizing, chairing, participating, and contributing to Workshops and Conferences, as well as reviewing papers and proposals for scientific journals and funding agencies

Two level-II milestones our group signed-on at the beginning of FY20 had been successfully completed

Status	Status Definition
G	Adequate - no significant issue
Y	Marginal - manageable schedule, technical or financial risk; can be accomplished
R	Inadequate - A serious or potentially unmanageable schedule, technical or financial risk
B	Complete

Task ID	Milestone title	Completion Criteria	RI	Status	Accomplishments
LLE10.8-22	Develop advanced and temperature-dependent exchange-correlation functionals to improve the prediction accuracy of transport and optical properties of HED plasmas using Density Functional Theory. (Q4 FY23).	Completion Criteria: This milestone is complete the newly developed temperature-dependent exchange-correlation functionals are shown to be a better description of materials properties of warm dense matter (typically in a published article).	Hu	B	This milestone is completed as planned. The temperature-dependent hybrid (KDT0) and meta-GGA (T-SCAN-L) exchange-correlation functionals have been developed and implemented into the QMD codes VASP and QE. A manuscript demonstrating the improvement of KDT0, when compared to PBE0, was published in Q3 [D. Mihaylov, V. V. Karasiev, S. X. Hu, Physical Review B 101, 245141 (2020).] Applications of T-SCAN-L to update LLE's FPEOS table of D2/DT have begun. The results obtained so far show that temperature-dependent exchange-correlation and quantum nuclear effects make D2/DT more compressible than previous models, which is in-line with the recent experimental evidence observed with LLNL reshock experiments [A. Fernandez-Pañella et al., Phys. Rev. Lett. 122, 255702 (2019)]. A manuscript reporting these new findings will be submitted to Physical Review B. This completes the planned work for FY20.
LLE10.8-23	Perform self-consistent DFT calculations of K α -emission in warm-/hot-dense matter to improve understanding of the atomic physics in HED plasmas. (Q4 FY20)	Completion Criteria: This milestone is complete when a manuscript, describing the comparison of predicted line-shifts with measured line-shifts (prior to FY20), has been prepare for peer-review journal submission.	Hu	B	This milestone is completed as planned. Exploratory DFT predictions of K α -emission in superdense plasmas have been completed. Two new phenomena were discovered: interspecies rative transition and dipole-forbidden K α -emission. The paper describing these findings was published in Q2 [S. X. Hu et al., Nature Communications 11, 1989 (2020)]. A code named "VERITAS" was under development during Q3 and Q4 for DFT-based non-LTE modeling of spherical spectroscopy experiments. The initial VERITAS simulations (of spherical spectroscopy experiments) have begun. The ultimate goal is to establish a platform/capability using K α and K β emission/absorption measurements to diagnose and understand the return shock and heat-wave propagation into a stagnating shell. A manuscript reporting the findings of extreme atomic physics in HED conditions is under preparation and will be submitted to Nature Physics soon. This completes the planned work for FY20.

Several accomplishments from HEDP-Theory Group had been highlighted in LLE's Report to NNSA/DOE



Key FY20 accomplishments

- TOP-9 experiments measured the impact of the Langdon effect (the creation of non-Maxwellian electron distribution functions) on CBET and confirmed long standing theory and ad hoc modeling of laser absorption in coronal plasmas.
- First experiments on the Fourth-generation Laser for Ultrabroadband eXperiments (FLUX) testbed demonstrated the feasibility of a novel frequency-conversion scheme from 1w to 3w in a nonlinear KDP crystal, resulting in efficient generation of UV pulses with fractional bandwidth larger than 1% (>9 THz).
- First-principles density-functional-theory (DFT) calculations revealed new interspecies radiative and non-dipole transitions in warm and superdense plasmas of heavy metals and their alloys.
- A new DFT-based molecular-dynamics calculation of warm dense hydrogen over a pressure range of 50 to 300 GPa confirms a metallic transition due to the dissociation of molecular hydrogen that coincides with an abrupt band gap closure.
- Experiments with the TOP9 platform confirmed that sufficiently large wavelength shifts will decouple the TOP9 beam from CBET with the OMEGA beams.
- During the two-month pandemic shutdown of the Omega Laser Facility, the operations staff developed a set of applications and protocols that allow fully remote experimental operations (the new capability is called "RemotePI").
- The HED Theory group updated the D2-FPEOS table using DFT calculations with a newly developed temperature-dependent SCAL-L exchange-correlation functional with quantum ion corrections.
- Laser heating of a gas in a cylindrical liner held in by a thin foil window (the MagLIF concept) was characterized as a function of time using spectrally integrated soft x-ray measurements.

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Key FY20 accomplishments

- LLE performed two experiments on the NIF to study the D_2 equation-of-state at pressures up to 1 TPa.
- Two-photon polymerization has been used to print nearly a dozen foam coated spherical capsules with a fill-tube.
- Power balance of the OMEGA laser (for 60-beam implosions) is routinely 3% for both sub-100-ps pickets and for arbitrary 100-ps windows of the main drive.
- Analysis of x-ray self-emission images from recent NIF PDD high adiabat implosions confirms that a contoured ablator can be used to correct the inherent polar drive asymmetry.
- First measurements with the Knock-On Deuteron imager (KoDI) demonstrated that the hot spot and the fuel shell can be imaged for high yield direct-drive DT implosions on OMEGA.
- Large-scale classical molecular dynamics simulations revealed that hydrogen ions stream ahead of the in-flight CH shell plasma confirming recent experimental measurements on OMEGA EP
- A HED investigation of thermal effects on the hP4 electrified phase of sodium (300-500 GPa) confirms that sodium can be classified as an insulator (not a semiconductor) in this phase and that upon melting becomes a metallic liquid.
- A methodology was developed to constrain the physics models (predictions) in convergent HED experiments by adapting Bayesian inference techniques (AI) for the analysis of limited experimental data.

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FY20 Awards for LLE personnel

- Ryan Rygg, the HEDPx group leader at LLE was elected a Fellow of the American Physical Society (APS).
- Jake Bromage, a Senior Scientist at LLE, was elected a Fellow of The Optical Society of America (OSA).
- Mike Campbell, the LLE Director, was elected a Fellow of the OSA.
- Sam Morse, the LLE Facility Division Director, was selected for Senior Membership in the OSA.
- Nick Savidis, the OMEGA EP System Scientist, was selected for Senior Membership in the OSA.
- The Fusion Power Associates Board of Directors has selected LLE staff scientist Dr.
- David Turnbull, a Scientist at the LLE, was awarded the 2020 FPA Excellence in Fusion Engineering Award.
- The APS Division of Plasma Physics and the European Physics Society (EPS) Plasma Physics Division recognized LLE Chief Scientist Riccardo Betti and LLE Senior Scientist Wolfgang Theobald with the Landau-Spitzer Award.
- Maitrayee Ghosh, LLE Horton Fellow, won the IBM-Zerner Graduate Student Award at the 60th Sanibel Symposium.
- Four students from the LLE 2019 Summer High School Research Program were selected as finalists in the [InspoScience Research and Innovation Competition](#) 2020 Virtual Edition.

Eight (8) first-authored papers have been published by HEDP-Theory Group members in 2020 (underlined authors)



1. R. Paul (Horton Fellow), S. X. Hu, V. V. Karasiev, S. A. Bonev, and D. N. Polsin, "Thermal effects on the electronic properties of sodium electride under high pressures", [Phys. Rev. B **102**\(9\), 094103 \(2020\)](#).
2. J. Hinz (Horton Fellow), V. V. Karasiev, S. X. Hu, M. Zaghoo, D. Mejia-Rodriguez, S. B. Trickey, L. Calderin, "Fully consistent density functional theory determination of the insulator-metal transition boundary in warm dense hydrogen", [Phys. Rev. Research **2**, 032065\(R\) \(2020\)](#).
3. D. I. Mihaylov, V. V. Karasiev, S. X. Hu, "Thermal hybrid exchange-correlation density functional for improving the description of warm dense matter", [Phys. Rev. B **101** \(24\), 245141 \(2020\)](#).
4. S. Zhang, S. X. Hu. "Species separation and hydrogen streaming upon shock release from polystyrene under inertial confinement fusion conditions", [Phys. Rev. Lett. **125**, 105001 \(2020\)](#).
5. S. X. Hu, V. V. Karasiev, V. Recoules, P. M. Nilson, N. Brouwer and M. Torrent, "Interspecies radiative transition in warm and superdense plasma mixtures", [Nature Communications **11**, 1989 \(2020\)](#)
6. S. Zhang, Michelle C. Marshall, Lin H. Yang, Philip A. Sterne, Burkhard Militzer, et al., "Benchmarking boron carbide equation of state using computation and experiment", [Phys. Rev. E **102**, 053203 \(2020\)](#).
7. S. Zhang, Heather Whitley, Tadashi Ogitsu. "Phase transformation in boron under shock compression", [Solid State Sciences, **108**, 106376 \(2020\)](#).
8. S. Zhang, Miguel Morales. "First-principles Equation of State and Structure of Liquid Metals at Multi-megabar Conditions", [AIP Conf. Proc. **2272**, 090004 \(2020\)](#).

Three (3) first-authored plus one co-authored manuscripts are ready for submission (by the end of 2020)



1. V.V. Karasiev, S.X. Hu, "*Unraveling the intrinsic atomic physics behind x-ray absorption line shifts in warm-dense silicon plasmas*", *Phys. Rev. E* (status: two positive Referee Reviews, will be re-submitted by the end of December 2020)
2. V. V. Karasiev, J. Hinz, S. X. Hu, and S.B. Trickey, "*Elucidation of the sub-critical character of the liquid-liquid transition in dense hydrogen*", *Nature*, Matters Arising (Status: this paper will be submitted to Nature by the end of December 2020).
3. S. X. Hu, R. Paul, V. V. Karasiev, R. P. Dias, "Carbon-doped sulfur hydrides as room-temperature superconductors at 270 Gpa", *Phys. Rev. Lett.* (to be submitted by 12/22/2020).
4. A. Shvydky, A. V. Maximov, V. V. Karasiev, D. Haberberger, and V. N. Goncharov, "*Ionization state and dielectric constant in cold rare fied CH plasmas of inertial con finement fusion*", *Phys. Rev. E* (Status: this paper is expected to be submitted by the end of December 2020).
5. (more to come in 2021)

HEDP-Theory Group members (underlined) contributed to **fifteen (15)** co-authored papers published in 2020



1. K. Luo , V. V. Karasiev, and S. B. Trickey, "Towards accurate orbital-free simulations: A generalized gradient approximation for the noninteracting free energy density functional", *Phys. Rev. B* **101**, 075116 (2020).
2. M. Millot, S. Zhang, D. Fratanduono, F. Coppari, S. Hamel, B. Militzer, D. Simonova, S. Shcheka, N. Dubrovinskaia, L. Dubrovinskaia, and J. Eggert. "Recreating giants impacts in the laboratory: Shock compression of MgSiO₃ bridgmanite to 14 Mbar", *Geophys. Res. Lett.*, **47**, e2019GL085476 (2020).
3. C. A. McCoy, S. X. Hu, M. C. Marshall, D. N. Polsin, D. E. Fratanduono, Y. H. Ding, P. M. Celliers, T. R. Boehly and D. D. Meyerhofer, "Measurement of the sound velocity and Grüneisen parameter of polystyrene at inertial confinement fusion conditions", *Phys. Rev. B* **102**, 184102 (2020).
4. Fionn D. Malone, S. Zhang, Miguel Morales. "Accelerating Auxiliary-Field Quantum Monte Carlo Simulations of Solids with Graphical Processing Units", *J. Chem. Theory Comput.* **16**, 4286 (2020).
5. A. Kar, S. X. Hu, G. Duchateau, J. Carroll-Nellenback, P. B. Radha, "Implementing a microphysics model in hydrodynamic simulations to study the initial plasma formation in dielectric ablator materials for direct-drive implosions", *Phys. Rev. E* **101**, 063202 (2020).
6. L. Lystrom, P. Tamukong, D. Mihaylov, S. Kilina "Phonon-Driven Energy Relaxation in PbS/CdS and PbSe/CdSe Core/Shell Quantum Dots", *J. Phys. Chem. Letters* **11** (11), 4269-4278 (2020).

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7. Burkhard Militzer, Felipe González-Cataldo, S. Zhang, Heather Whitley, Damian Swift, and Marius Millot. “Nonideal Mixing Effects in Warm Dense Matter Studied with First-Principles Computer Simulations”, [J. Chem. Phys. 153, 184101 \(2020\)](#).
8. A Pineau, B Chimier, S. X. Hu, G Duchateau, “*Modeling the electron collision frequency during solid-to-plasma transition of polystyrene ablator for direct-drive inertial confinement fusion applications*”, [Phys. Plasmas 27, 092703 \(2020\)](#).
9. V. N. Goncharov, I. V. Igumenshchev, D. R. Harding, S. F. B. Morse, S. X. Hu, P. B. Radha, D. H. Froula, S. P. Regan, T. C. Sangster, E. M. Campbell, “*Novel Hot-Spot Ignition Designs for Inertial Confinement Fusion with Liquid-Deuterium-Tritium Spheres*”, [Phys. Rev. Lett. 125, 065001 \(2020\)](#).
10. D. Fratanduono, R. Smith, S. Ali, D. Braun, A. Fernandez-Pañella, S. Zhang, R. Kraus, F. Coppari, J. McNaney, M. Marshall, L. Kirch, D. Swift, M. Millot, J. Wicks, and Jon Eggert. “Probing the Solid Phase of Noble Metal Copper at TPa Conditions”, [Phys. Rev. Lett., 124, 015701 \(2020\)](#). ([LLNL newslines](#)).
11. Joseph Nilsen, Daniel Åberg, Heather Whitley, Brian Wilson, Lin Yang, Philip Sterne, Markus W. Daene, Madison Martin, S. Zhang, and Walter R. Johnson. “Role of opacity at the 9 keV back lighter energy used in measuring the equation of state of boron at pressures up to a Gbar”, [High Energ. Dens. Phys., 37, 100880 \(2020\)](#).
12. P. R. C. Kent, Abdulgani Annaberdiyev, Anouar Benali, ..., Shiv Upadhyay, Hongxia Hao, Guangming Wang, S. Zhang, Luning Zhao. “*QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion Quantum Monte Carlo*”, [J. Chem. Phys. 152, 174105 \(2020\)](#). (Editor's Pick)



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13. L Ceurvorst, R Betti, A Casner, V Gopalaswamy, A Bose, S. X. Hu, EM Campbell, et al., “Hybrid target design for imprint mitigation in direct-drive inertial confinement fusion”, *Phys. Rev. E* 101, 063207 (2020).
14. Burkhard Militzer, Felipe González-Cataldo, S. Zhang, Kevin Driver, François Soubiran. “First-principles equation of state database for warm dense matter computation”, *Phys. Rev. E, in press*. (<https://arxiv.org/abs/2012.07093>).
15. PE Grabowski, SB Hansen, MS Murillo, LG Stanton, FR Graziani, ..., Y Hou, S. X. Hu, D Jensen, ..., A White, “Review of the first charged-particle transport coefficient comparison workshop”, *High Energy Density Physics* 37, 100905 (2020).

Close collaborations with HEDx, IM, and Implosion-Experiment Groups have been strengthened in 2020



- **Joint HED-xt Meeting has been established for closer collaborations**
- **Eight collaborative projects are on-going between HEDt and HEDx /IM Groups:**
 - **MgO melting and other HED behaviors (S. Zhang, L. Crandall B. McLellan,...)**
 - **Extreme atomic physics at Gbar pressures (S. X. Hu, P. Nilson, V.V. Karasev,....)**
 - **Double shock in CH (M. Ghosh, Z. Sprowal, ...)**
 - **Super-hard materials with Boron (S. Zhang, D. Polsin,....)**
 - **Cone-in-double-shell platform (S.X. Hu, R. Rygg, W. Theobald, D. Polsin, ...)**
 - **Shock release at CH/DT interface (S. Xhang, M. Marshall,....)**
 - **Understanding refractive index of release plasmas (V. Karasev, A. Shvydky,...)**
 - **Laser imprint understanding/mitigation (S. Hu, J. Peebles, W. Theobald, S. Regan,....)**
- **Five jointed HEDxt papers published or submitted in 2020 (more to come):**
 - **Melting and electron bubble of Na (PRB - published)**
 - **H2/D2 insulator-metal transition (PRR - published)**
 - **Hugoniot and sound-speed of Si (PRB - submitted)**
 - **Inter-species radiative transition (Nature Communication – published)**
 - **Gruneisen parameter and sound speed of CH (PRB – published)**

Collaborations with National Labs and other Universities are healthy, active, and productive

- **Collaborations with LANL on three fronts are on-going well:**
 - ❑ With L. A. Collins & A. White on TD-DFT development for stopping power (S. Hu)
 - ❑ With M. Schmitt & B. Scheiner on double-shell (S. Hu)
 - ❑ With C. Starrett & N. Shaffer on transport and WDM (S. Hu, S. Zhang)
- **Collaborations with LLNL are fruited in the following projects:**
 - QMC simulation of materials with M. Morelas (S. Zhang)
 - Melting of Sn (S. Zhang,...)
 - Meta-dynamics and HED-material phases (R. Paul, S. Hu, S. Bonev: one jointed PRB)
- **Collaboration with SNL on extreme atomic physics is expected to fruition soon (S. Hu, P. Nilson, S. Hansen)**
- **Collaboration with CELIA and CEA had resulted in three jointed papers (S. Hu, V. Karasev, V. Recoules, G. Ducheateau, A. Pineau)**
- **Collaborations with U. Florida (V. Karasev, S. Trickey), UC-Berkeley (S. Zhang, B. Militzer), U. Buffalo (E. Zurek, S. Zhang), PPPL (S. Hu, W. Fox), Princeton (S. Zhang + T. Duffy), Imperial College (S. Hu, M. Ghosh, G. Kagan) are strong and productive.**

Graduate Students in HEDP-Theory Group are making great progress towards their educational goal



- Reetam Paul has successfully passed his PhD Qualifying Exam in August 25, 2020. Now, he is a *PhD Candidate* at Department of Mechanical Engineering (UoR); will graduate one year from now!
- Josh Hinz has also successfully passed his PhD Qualifying Exam in October 20, 2020. Now, he is a *PhD Candidate* at Department of Physics & Astronomy (UoR)!
- Matrayee Ghosh won the IBM-Zerner Graduate Student Award at the 60th Sanibel Symposium in Feb. 2020! She is making progress towards publishing her first paper on HED-Chemistry in 2021(?).
- Brenda McLellan is actively working on her project of figuring out the phase transition pathway for MgO under high-pressure loadings, that may lead to her first paper in 2021(?).
- One or two more PhD student(s) may join our group in 2021(?)

HEDP-Theory Group members have actively served the broad physics community in 2020



- **V. Karasev** refereed papers for PRL/PRB/PRE... and reviewed proposals for DOE/NSF
- **S. Zhang** refereed papers for PRB/PRE/....
- **S. Zhang and V. Karasev** participated and contributed to ICF-2030 Workshop: Materials Working Group
- **D. Mihaylov, J. Hinz, B. McLellan, S. Zhang, V. Karasev, and S. Hu** presented talks at APS-DPP-2020
- **S. Hu** served the ICF sub-committee for APS-DPP-2020, chaired two sessions there; co-organized ICF-2030 Workshop: Materials Working Group; refereed papers for Nature-Communication/PRL/PRA/PRE/HEDP; and reviewed proposals for DOE
- **S. Zhang** presented at AGU meeting 2020

External Grants to Work on

- **V. Karasev (PI), D. Mihaylov, & S. Hu (Co-PI) continued working on our NSF Grant PHY-1802964. Renewal of this grant will be planned in 2021.**
- **V. Karasev (PI) were awarded 3.5 Millions of Hours on NERSC Supercomputer at Berkeley.**
- **S. Hu (Co-I) started to be part of the NSF's Physics Frontier Center Award: Center for Matter at Atomic Pressure (CMAP) [2020-2025]**

Summary



"On the other hand, it's been a great year for HED-t

" LOOKS LIKE THE BAR
HAS BEEN RAISED."

