A Machine Learning Study of Properties of D_2O up to 8 Million Kelvin from First Principles

Strongly Coupled Coulomb Systems 2025

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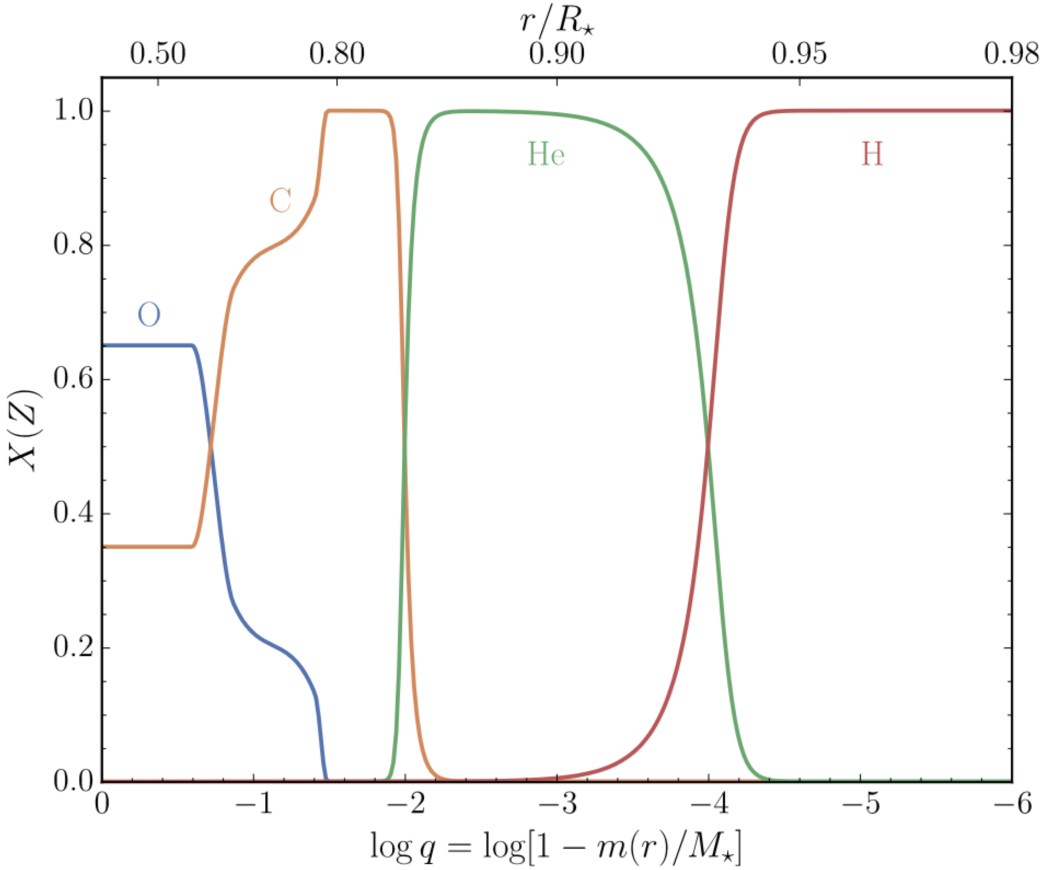
White Dwarf Stars

- The fate of the vast majority of stars (including the Sun) is a White Dwarf (WD)

- Cooling rate depends on:
  - Neutrino production rate in the core
  - Thermal conductivity in the core and envelope
  - Radiative opacity in the atmosphere
  - Element transport in the interior
  - Physics of phase transition

- WD stars can serve as cosmic clocks

“Core”

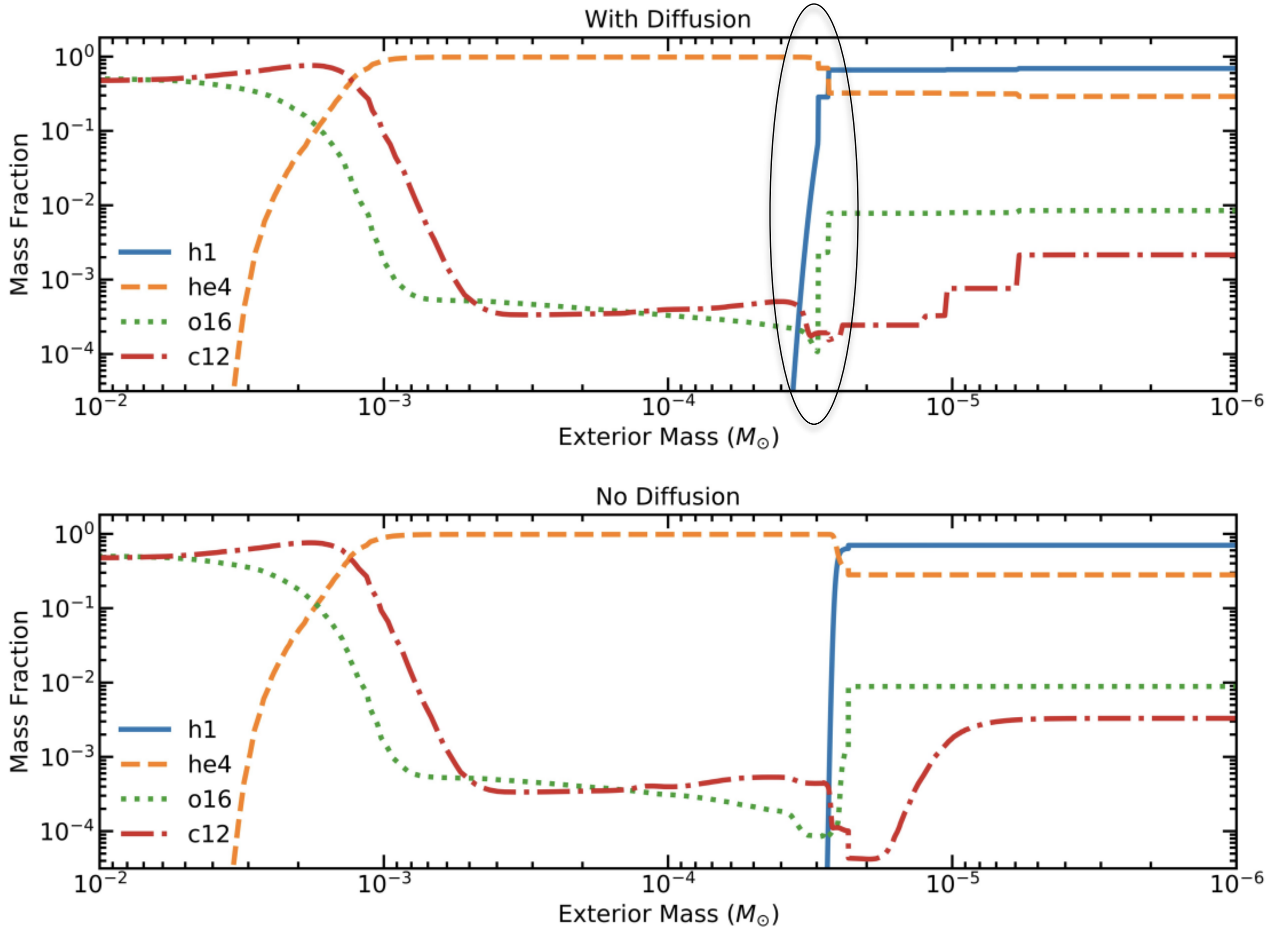


“Surface”

Physics Reports, 988, 1-63 (2022)

Transport Coefficients of White Dwarf Stars

White Dwarf Model



- The astrophysics of WD stars is a mature field with a wealth of observations calling for refined physics models

- Many processes in WD models in the partially ionized surface remain difficult to model

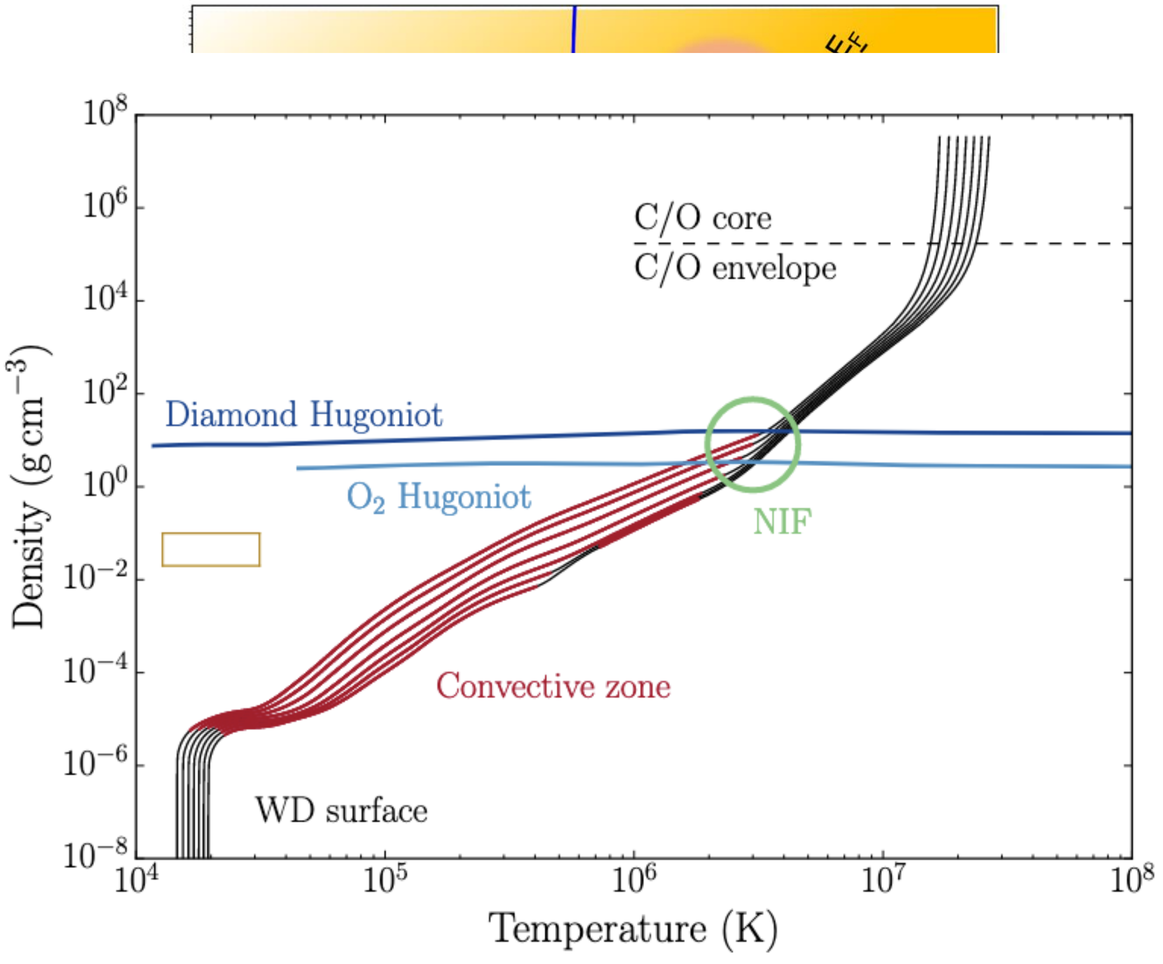
  - When diffusion is enabled for this 1D-WD model, the hydrogen layer is able to penetrate further into the star.

Wilhite, H., and Wolf, W. *Modeling Diffusion in Accreting White Dwarf Stars*, UW Eau Claire, 2021

Equation of State (EOS) of WD Stars

- EOS for matter in the less dense, partially ionized surface zone of a WD star is *not well understood*
- Pressures of ~ 1 Gbar on the principal Hugoniot correspond to the ionization of the K electronic shells of C and O
- Pressure in EOS tables used in white dwarf models can differ by 40% in this regime

Recent NIF experiments probing D_2O EOS motivate our efforts to provide precise theoretical estimates of EOS and transport properties.



Density ρ (g/cm^3)

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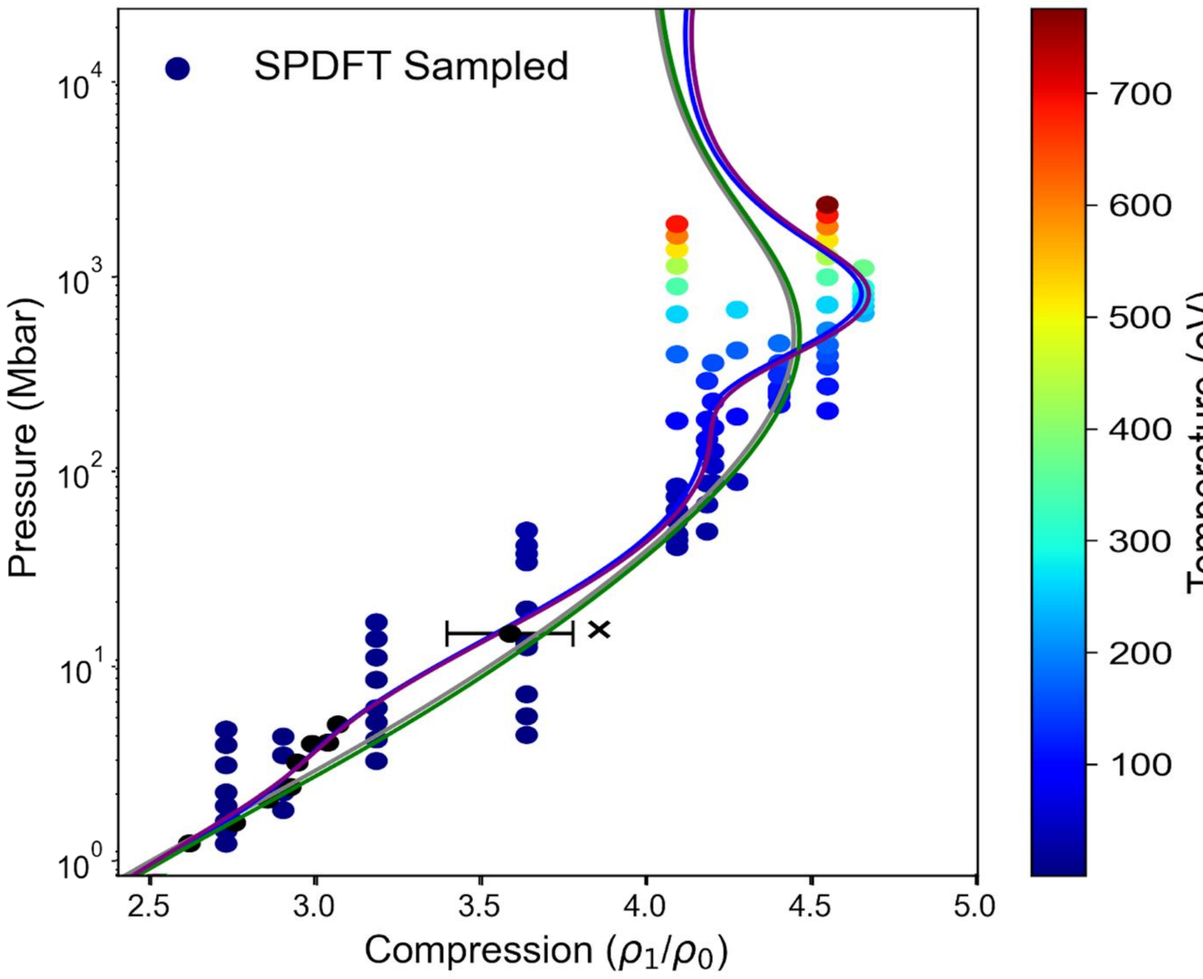
Ab initio Molecular Dynamics

- Ab initio simulations of plasmas represent the current state-of-the-art for calculating EOS and transport properties (but *computationally intensive*)

- We leveraged the LLNL-developed KS-DFT code (SPARC) and its Spectral Partitioning implementation

- Carried out DFT-MD simulations of D_2O using the PBE XC functional for systems of 81 atoms under the NVT ensemble



Sadigh *et al.*, PRE 108, 045204 (2023)

EOS Properties

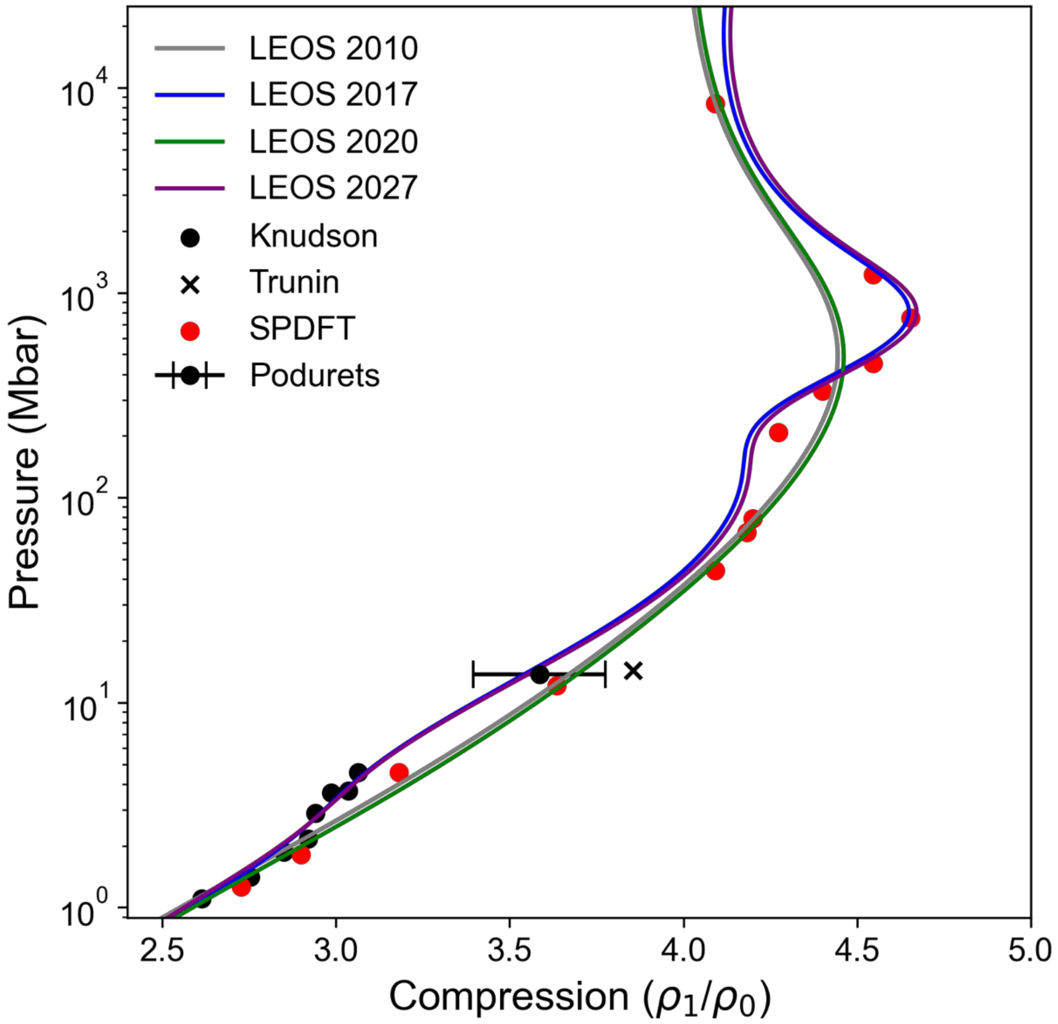
Rankine-Hugoniot Equations

$$\rho(u_s - u_p) = \rho_0 u_s$$

$$P - P_0 = \rho_0 u_s u_p$$

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$

- Our simulations shows a good agreement with Livermore EOS (LEOS) 2027/2017 suggesting that Thomas-Fermi model is not sufficient for an accurate EOS model of D_2O

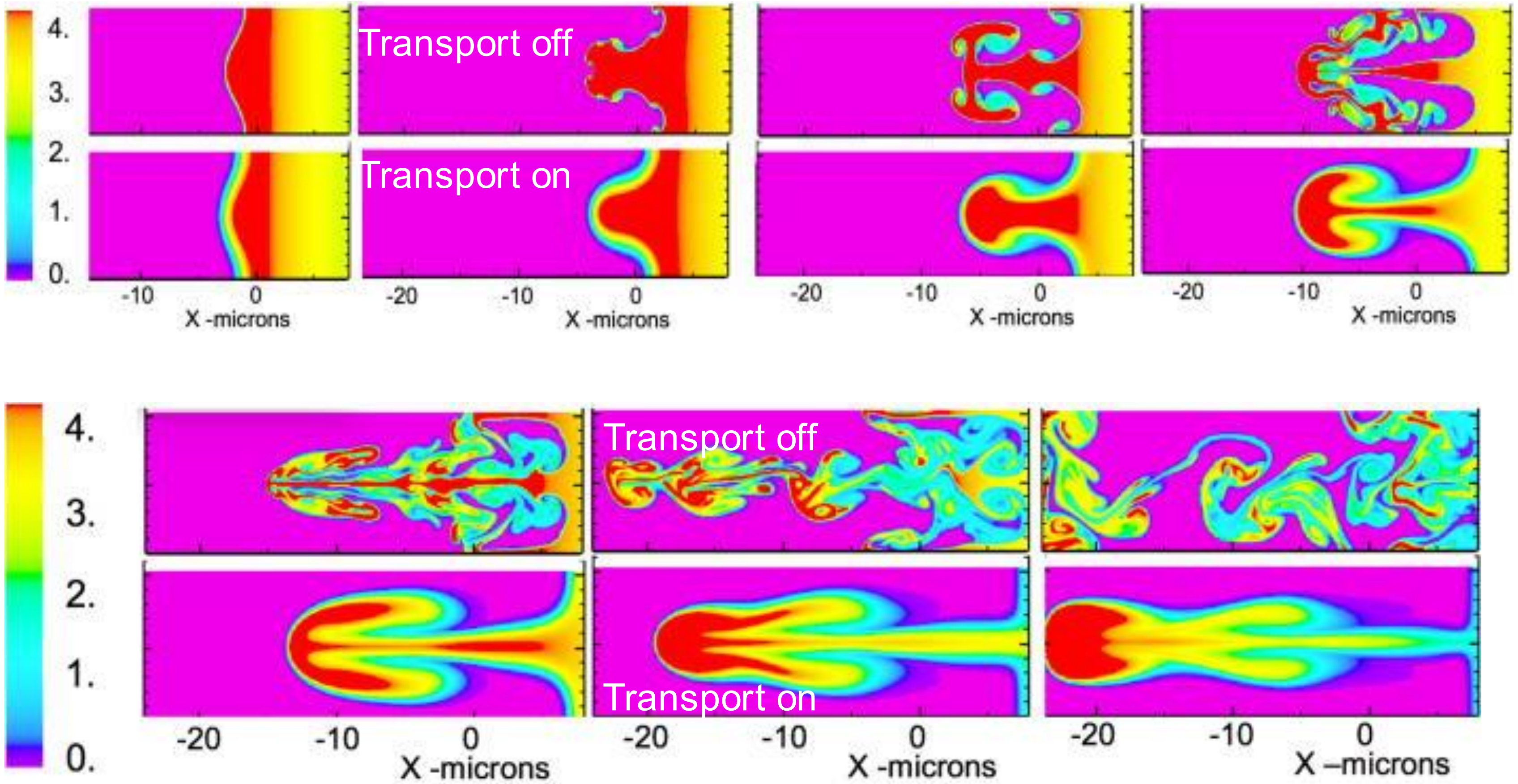


Hydrodynamic Simulations

Hydrodynamic Simulations of Rayleigh-Taylor instability with and without plasma viscosity and diffusivity show:

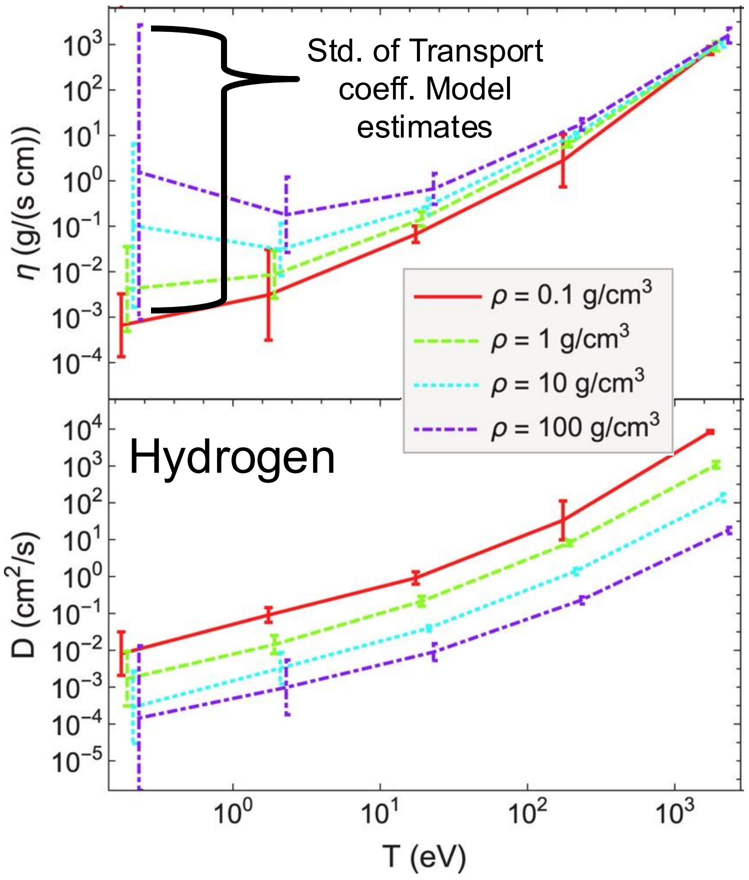
- Plasma transport smooths flow fields
  - Reduces small-scale structure
- Reduces instability growth

Accurate transport coefficient estimates are essential



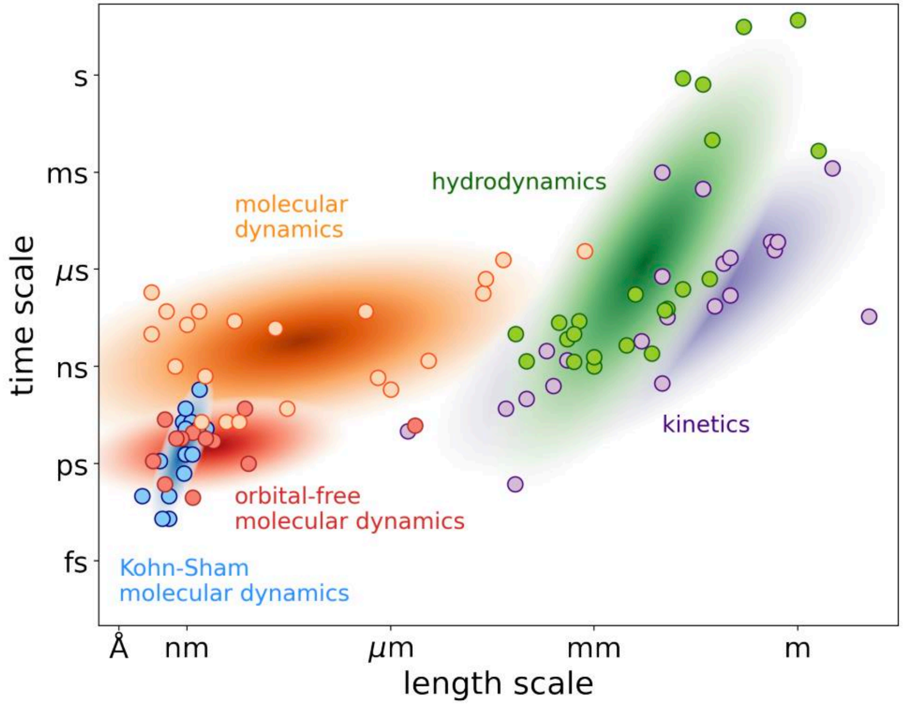
Phys. Plasmas 31, 043905 (2024)

Transport Coefficient Models



- Warm dense matter transport coefficient models are fit for strongly coupled systems

- Transport coefficient models estimates have shown variation up to 6 orders of magnitude



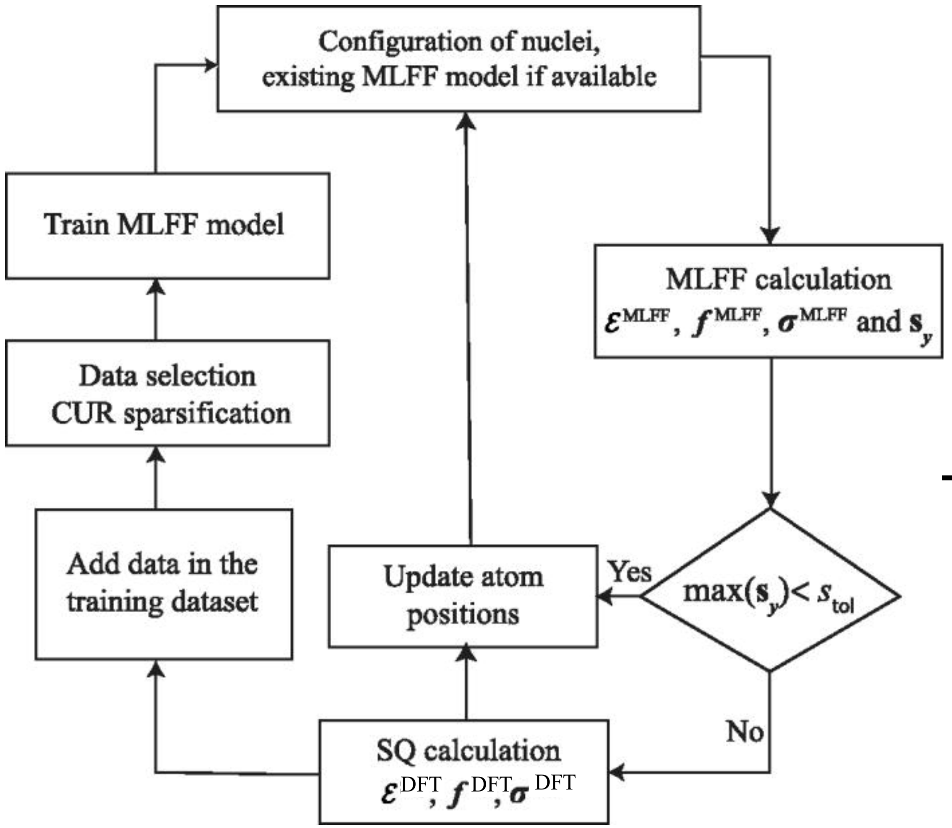
- MD simulations can provide plasma transport coefficients in both weakly and strongly coupled regimes

P.E. Grabowski, et al. *High Energy Density Phys.* 37, 100905 (2020)

L. Stanek. Computational Methods for Nonideal Plasmas, Michigan State University (2022)

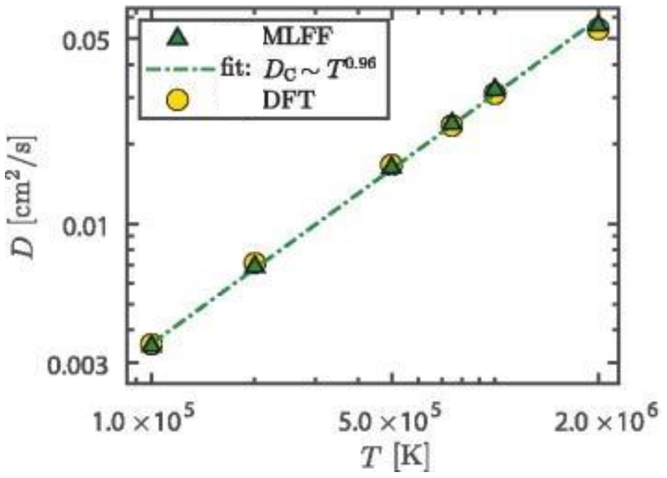
"On the Fly" Machine Learned Interatomic Potentials (MLIP's)

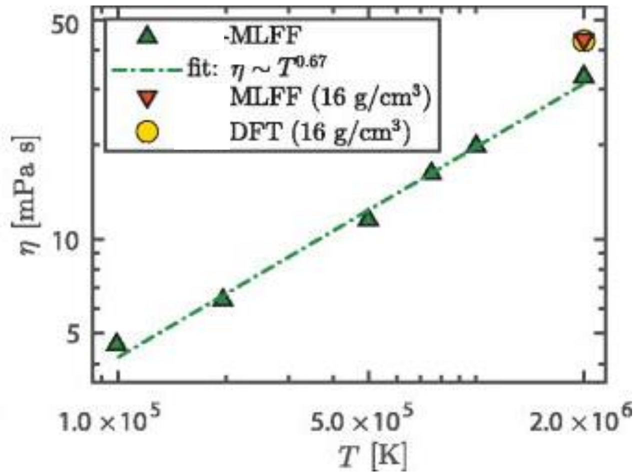
KS-DFT MLFF Framework



MLIPs were developed "on-the-fly" to capture the complexity of the system for a wide range of conditions at varying ionization states

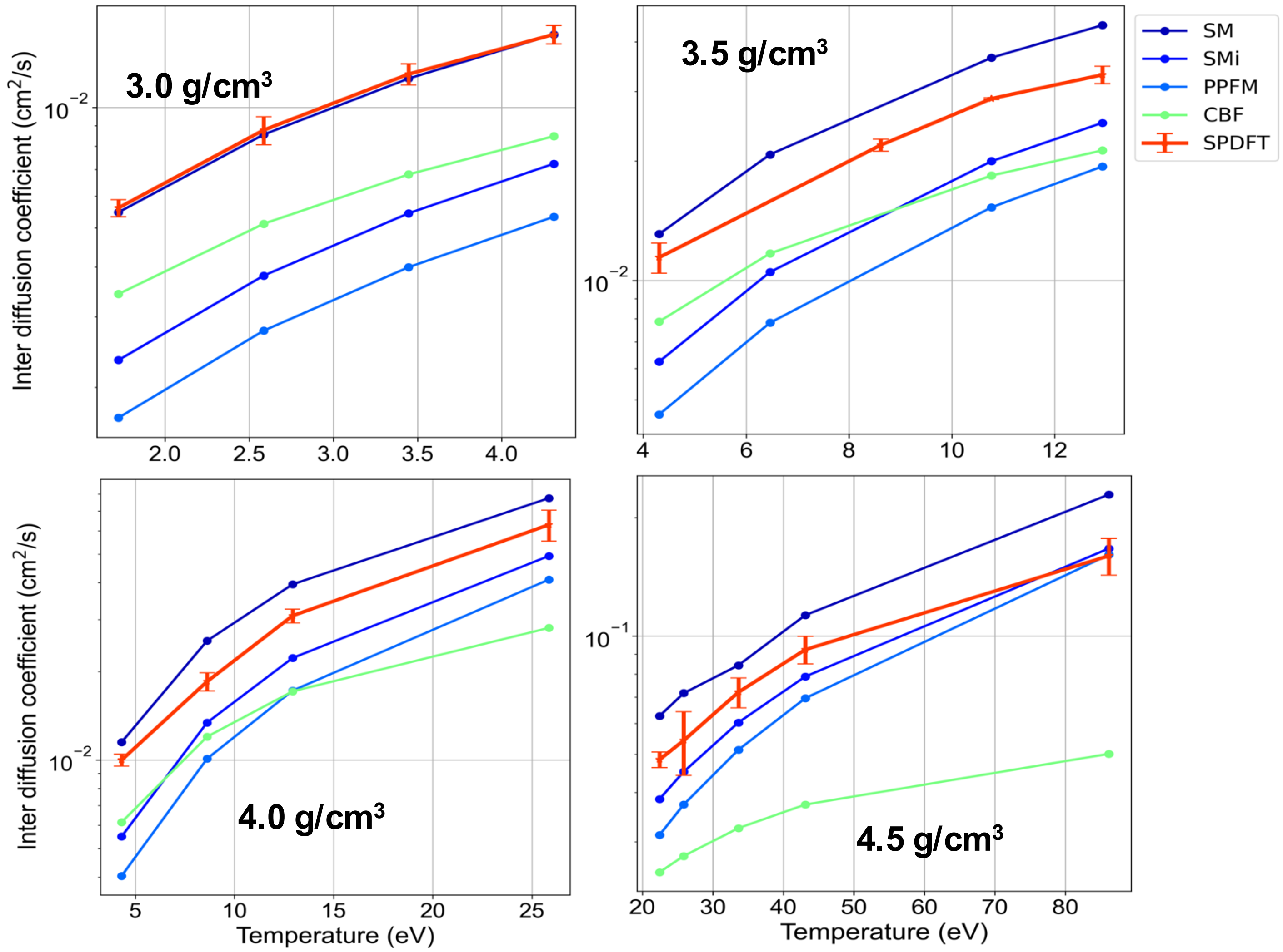
The KS-DFT Machine Learned Force Fields (MLFF) framework has previously shown good agreement with KS-DFT transport coefficient estimates





Kumar *et al*., arXiv.2402.13450

Interdiffusion



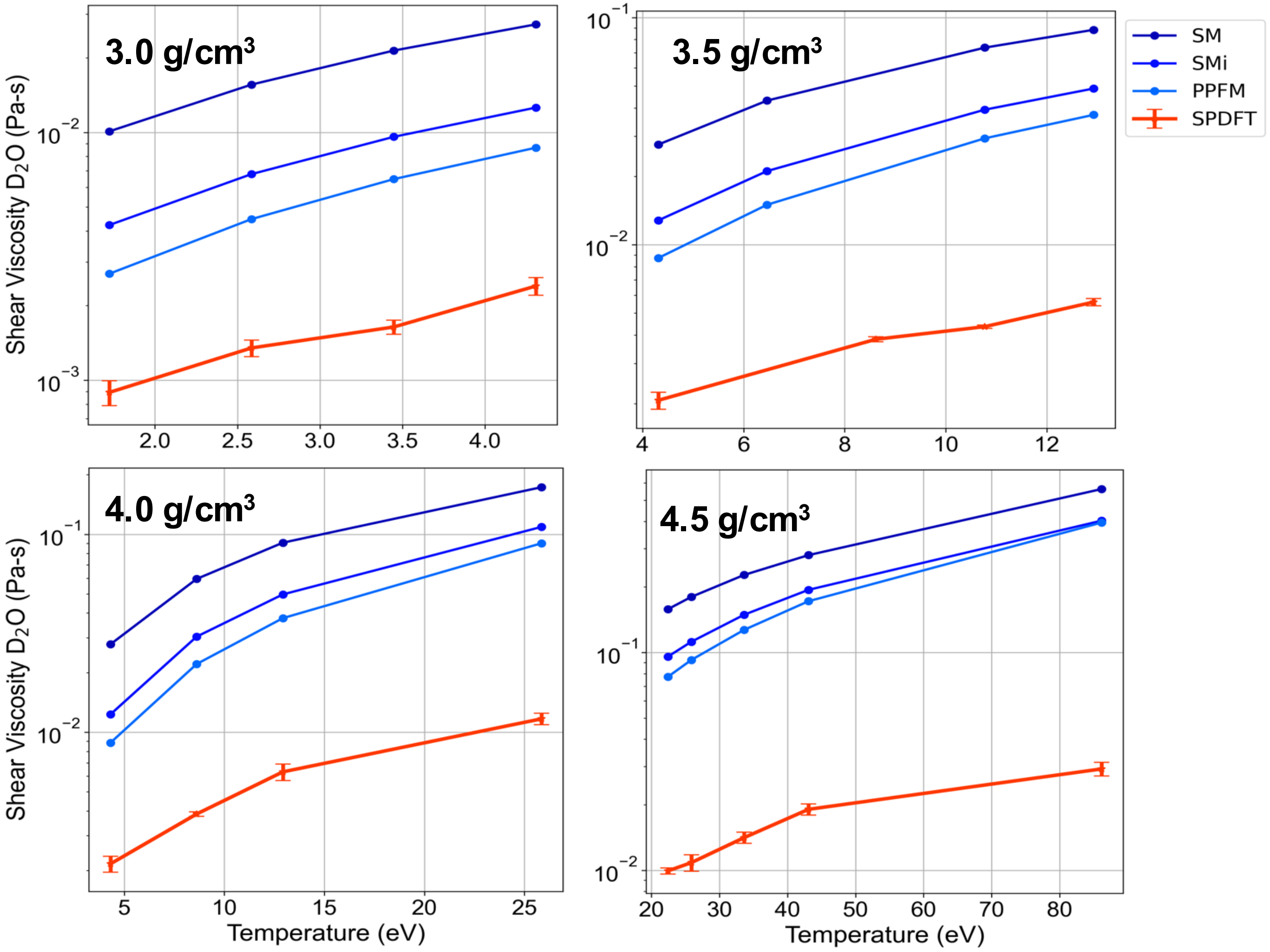
Atomic scale mixing between species is described through terms that contains the inter-diffusion coefficient D_{12} :

$$D_{12} = \frac{J}{3Nx_1x_2} \int_0^\infty \langle \mathbf{j(t)} \cdot \mathbf{j(0)} \rangle \mathbf{dt}$$

$$\mathbf{j(t)} = \mathbf{x_2} \sum_{\mathbf{i=1}}^{\mathbf{N_1}} \mathbf{v_{1,i}(t)} - \mathbf{x_1} \sum_{\mathbf{i=1}}^{\mathbf{N_2}} \mathbf{v_{2,i}(t)}$$

For all sampled temperatures and densities, the SPDFT results were in the best agreement with the Stanton Murillo transport model

Viscosity



The shear viscosity can be calculated by integrating the shear stress autocorrelation function:

$$\eta = \frac{V}{5k_B T_i} \int_0^\infty dt \sum_{i=1}^{5} \langle \boldsymbol{\sigma}_i'(0) \cdot \boldsymbol{\sigma}_i'(t) \rangle$$

$$\boldsymbol{\sigma}' = \left[\sigma_{12}, \sigma_{23}, \sigma_{31}, \frac{(\sigma_{11} - \sigma_{22})}{2}, \frac{(\sigma_{22} - \sigma_{33})}{2} \right]$$

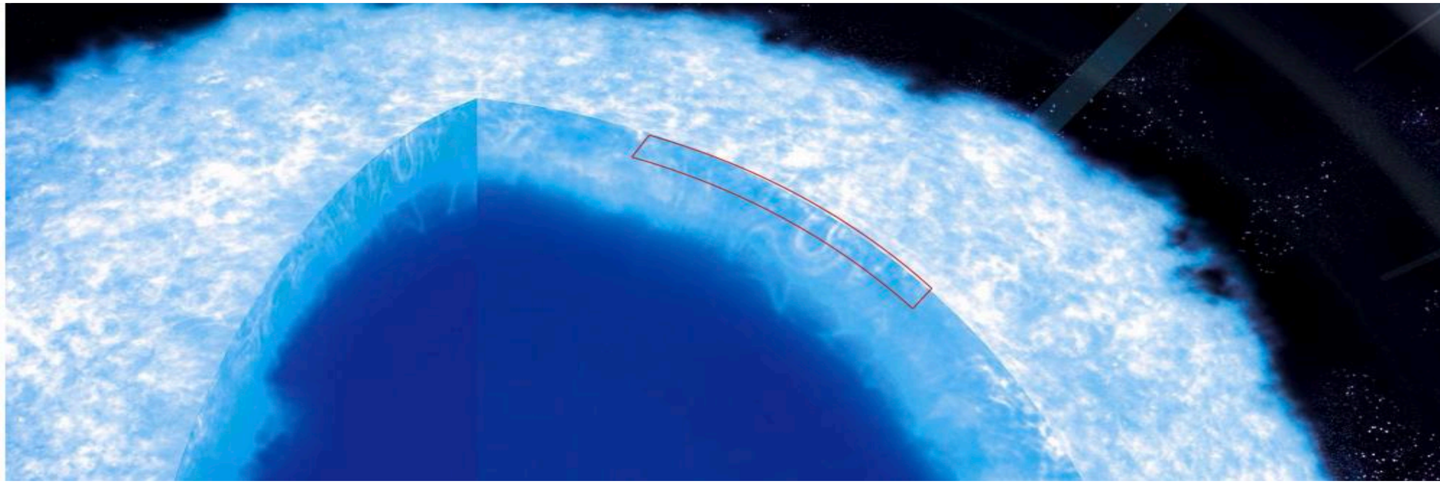
As density increases the difference between the viscosity predictions of the transport models and SPDFT grows to one order of magnitude

Conclusions

- Our work showcases the capabilities of SPARC to efficiently sample EOS and transport properties of a system at White Dwarf relevant conditions
- LEOS tables (that account for shell structure) accurately reproduce KS-DFT predicted EOS properties for D_2O
- Transport coefficient models accurately reproduce interdiffusion coefficients but show large deviation in viscosity

Future Work

- Determine source for large discrepancies in viscosity between transport coefficient models and KS-DFT
- Determine the impact of small and large discrepancies in transport coefficients on the results of hydrodynamic simulations for various applications



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