

# Data-driven Surrogate Modeling of Matter under Extreme Conditions

*Monday 6 December 2021 10:10 (20 minutes)*

The successful diagnostics of phenomena in matter under extreme conditions relies on a strong interplay between experiment and simulation. Understanding these phenomena is key to advancing our fundamental knowledge of astrophysical objects and has the potential to unlock future energy technologies that have great societal impact.

A great challenge for an accurate numerical modeling is the persistence of electron correlation and has hitherto impeded our ability to model these phenomena across multiple length and time scales at sufficient accuracy. In this talk, I will present a solution to this problem in terms of a data-driven modeling framework for matter under extreme conditions –the Materials Learning Algorithms (MALA) package. MALA generates surrogate models based on deep neural networks that reproduce the output of state-of-the-art electronic structure methods at a fraction of their computational cost. This opens up the path towards multiscale materials modeling for matter under ambient and extreme conditions at a computational scale and cost that is unattainable with current algorithms.

MALA is jointly developed by the Center for Advanced Systems Understanding (CASUS) at the Helmholtz-Zentrum Dresden-Rossendorf, Sandia National Laboratories (SNL), and Oak Ridge National Laboratory (ORNL).

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## Physical Presentation

I would be willing present physically.

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