

Marius Stan, Ph. D.

Dr. Marius Stan is a computational chemist and physicist interested in non-equilibrium thermodynamics, heterogeneity, and materials design for energy and electronics applications. He uses artificial intelligence, machine learning, and multi-scale computer simulations to understand and predict properties of materials.

Marius was born in Romania and graduated with a B.S. in Physics from the University of Bucharest, Department of Physics. In 1997 he received the Ph. D. in Chemistry from the “Ilie Murgulescu” Institute of Physical Chemistry of the Romanian Academy. The same year he joined Los Alamos National Laboratory in the United State of America as a postdoctoral research associate. Shortly after he become a permanent scientist and created and led a research group on computational chemistry and physics of materials. In 2010, Marius joined Argonne National Laboratory in Chicago as a Senior Computational Energy Scientist. He is also Adjunct Professor and Senior Fellow at the University of Chicago’s Computation Institute and at the Northwestern-Argonne Institute for Science and Engineering.

The goal of Marius’ research is to discover or design materials, structures, and device architectures for energy and electronics applications, such as nuclear fuels, battery electrodes, and materials for the new generation computers. To that end, Marius and his group develop theory-based (as opposite to empirical) mathematical models of chemical and thermodynamic properties of imperfect materials. The imperfections come from defects or deviations from stoichiometry (e.g., in battery electrodes), from irradiation (e.g. in nuclear fuels), or doping (e.g. computer memory devices). Then they use the models in computer simulations of coupled heat and chemical transport, micro(nano)-structure evolution, phase-stability, and phase transformations. To analyze large and complex experimental and computational data sets, the group uses Bayesian analysis, artificial intelligence, and machine learning methods based on regression and evolutionary (genetic) algorithms that can produce robust data screening and sampling. In parallel, they design experiments to validate the models and simulations.

Marius has recently completed an Intergovernmental Personnel Act (IPA) appointment with the U.S. Department of Energy Office of Nuclear Energy (DOE-NE). An IPA permits the temporary assignment of skilled scientists or engineers to positions within federal agencies. Marius served as Senior Advisor for modeling and simulation to the Assistant Secretary for DOE-NE and as National Technical Director for the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. As director of the NEAMS program, Marius coordinated activities with the DOE energy innovation hubs and represented DOE-NE in interactions with programs in the Office of Science and the National Nuclear Security Administration.

Over the last two decades, Marius developed an international strategy for the Organization for Economic Cooperation and Development (OECD) – the Nuclear Energy Agency (NEA) that resulted in a working party on multiscale models and simulation for nuclear energy and five international expert groups involving eighteen OECD countries. In 2002, he created the Materials Models and Simulations for Nuclear Fuels (MMSNF) workshop series that defined and promoted the concepts of “multi-scale models and simulations”, a methodology that is now being used worldwide for materials design.

Marius’ current projects include: “thermodynamics of imperfect materials”, focused on atomically engineering defects in materials for electronics; “heterogeneity by design,” a study of heterogeneous (non-uniform) materials that have improved properties compared to the homogenous ones; and “ZOOM,” a multiscale computational microscope that can “focus” at various time and length scales using as “lenses” computational methods. Marius has extensively published in the scientific literature and is writing a book on “Models and Simulations of Materials” for Taylor & Francis. He is a published author of short-stories and poetry (in Romanian), and an actor that you may recognize as *Bogdan* in the acclaimed TV series “Breaking Bad.”