**Multitasking neural networks for first-principles based statistical mechanics of alloys and magnetic systems**

Massimiliano Lupo Pasini, Markus Eisenbach, Junqi Yin, Ying Wai Li, Jiaxin Zhang

Oak Ridge National Laboratory

[lupopasinim@ornl.gov](mailto:lupopasinim@ornl.gov)

**Abstract**

Computing the thermodynamics of alloys and magnetic systems via first principles calculations can become computationally expensive as the system size increases. Reducing the computational cost thus becomes essential. We tackle this problem by constructing highly accurate surrogate models to estimate physical quantities using neural networks for nonlinear regression. In particular, we perform joint training of neural networks to predict multiple physical quantities such as total energy, charge density, and magnetization simultaneously. Our numerical experiments show that this practice improves the predictive power of the regression model. In addition, there is a strong correlation between the total energy of a solid crystal structure and the other physical properties like charge density and magnetization. This strong correlation acts as a physical constraint during the training process, which helps eliminate numerical artifacts like overfitting and leads to more reliable prediction.