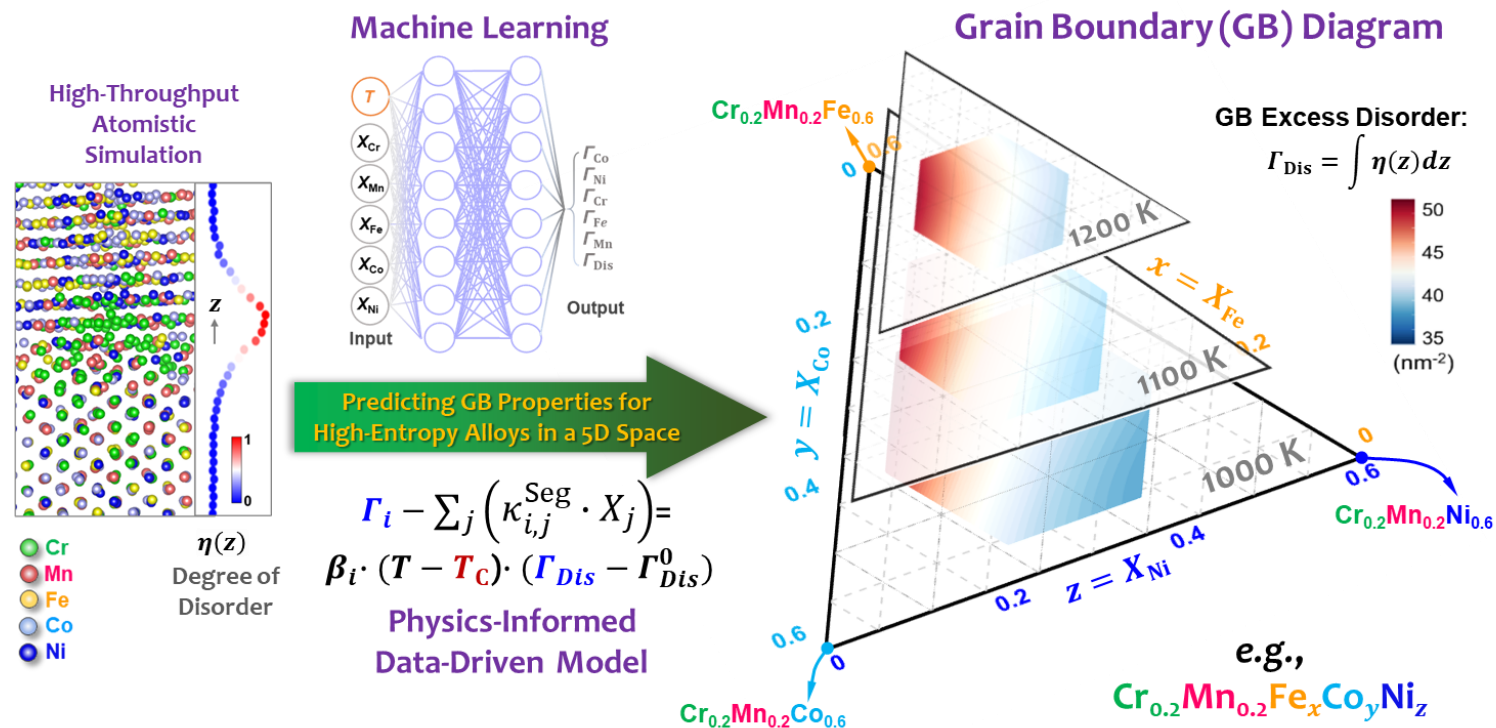


# Data-Driven Prediction of Grain Boundary Segregation and Disordering in High-Entropy Alloys in a 5D Space

Jian Luo, University of California, San Diego

- We combine large-scale atomistic simulations and machine learning to predict the properties of grain boundaries (GBs) in high-entropy alloys (HEAs) as functions of four independent compositional degrees of freedom and temperature in a 5D space.
- GB diagrams can be constructed.
- A data-driven discovery further reveals new coupled GB segregation and disordering effects in HEAs, uncovering new phenomena beyond the classical GB segregation models.
- A physics-informed data-driven model is constructed to provide more physical insights and better transferability.
- Further collaboration within IRG-1 groups will examine the predictions experimentally.
- The ability to predict GB properties in a 5D space for HEAs represents a new paradigm.



Chongze Hu, Jian Luo, *Materials Horizons*, 9: 1023–1035 (2022)

<https://doi.org/10.1039/d1mh01204e>