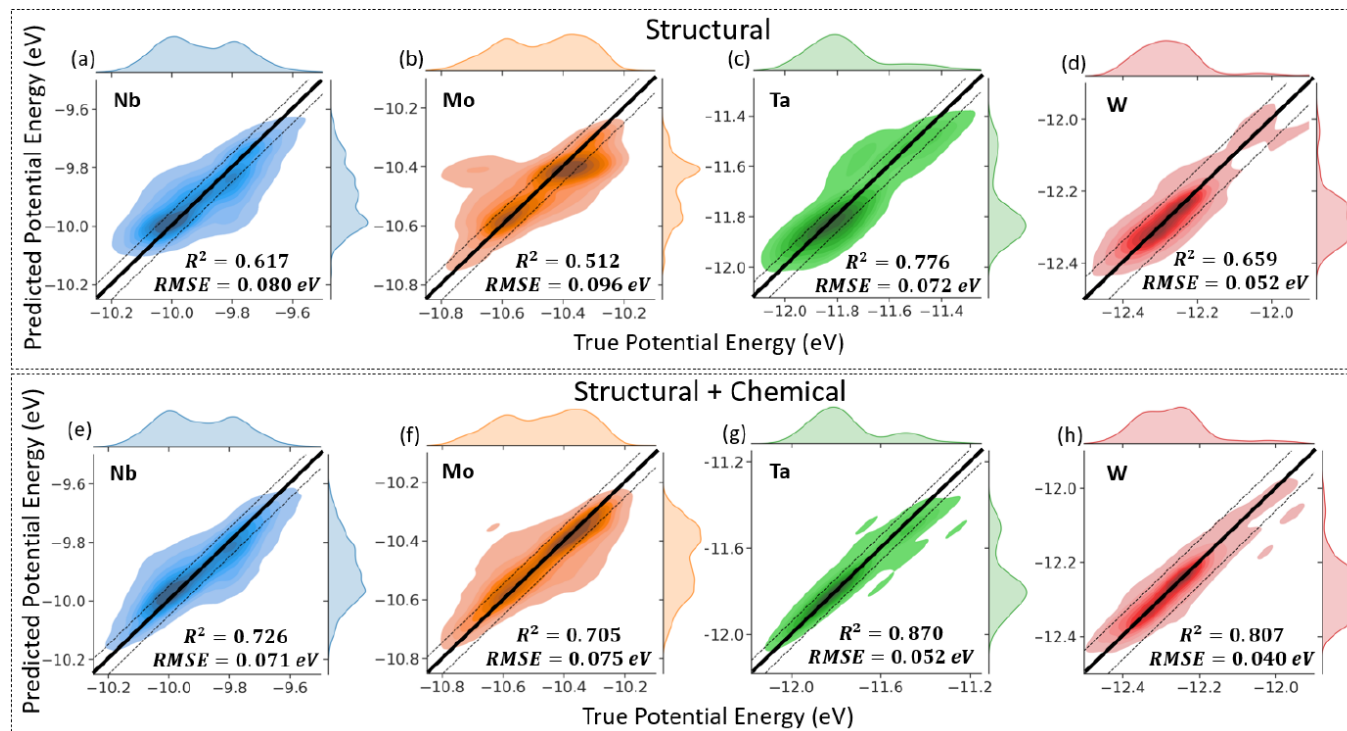


# High-throughput simulations demonstrate the importance of local chemistry for interfacial segregation in NbMoTaW

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High-throughput atomistic models were used to study interfacial segregation in a NbMoTaW refractory complex concentrated alloy. Hundreds of bicrystals and hundreds of thousands of atomic grain boundary sites were tested. Nb was found to be the dominant segregant, but important deviations from this average response highlighted the unique behavior of complex concentrated alloys. For example, incomplete Ta depletion was observed when these elements were frozen into the grain boundary by nearby Mo atoms, showing the importance of chemical ordering.

Machine learning models capturing the structural and chemical features of interfacial sites were used to weigh their relative contributions to segregation. A significant increase in predictive capability was observed when including local chemical information. This study pushed the IRG closer to its goal of being able to predict grain boundary structure and chemistry in complex concentrated materials.



Results of machine learning (random forest model) analysis of the energy for grain boundary sites in NbMoTaW. The predictions dramatically improve when both structural and chemical features are used.

Geiger I, Luo J, Lavernia EJ, Cao P, Apelian D, Rupert TJ. "Influence of chemistry and structure on interfacial segregation in NbMoTaW with high-throughput atomistic simulations," *Journal of Applied Physics*, **132**, 235301 (2022). <https://doi.org/10.1063/5.0130402>

