Effect of atomic distribution in alloys on the Interfacial Force Fields.

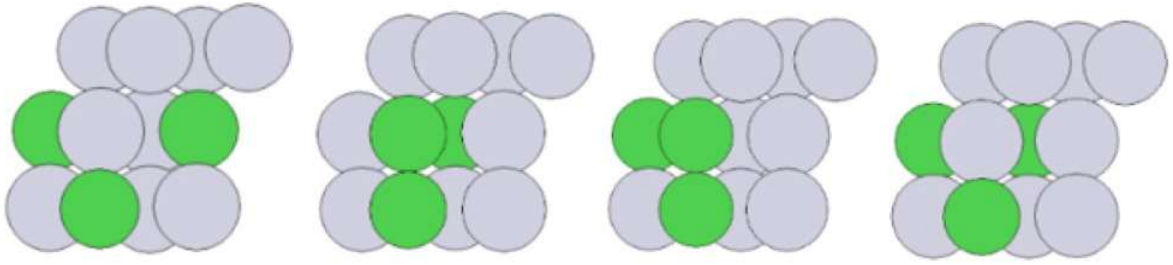
Simulation	X	Modelling	X
Experiment	O	Construction	O

Motivation

- Interfacial force fields (IFF), used in Molecular Dynamics (MD) Simulations are critical in understanding interactions in multiphase systems.
- Alloy materials in multiphase systems such as aircraft fuel cells, make the IFF case sensitive and hence less transferable.
- We would like to observe the effects of atomic distribution on IFF parameters.

Questions

- Ab initio Simulations for training dataset generation.
- MD Simulations for parameter optimization.



We are looking for students who are motivated to learn and implement Molecular Simulations for thesis and master's theses.

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