# From DFT to precipitation and strengthening in Aluminum Alloys

**A. Jain[1], D. Marchand[1], Y. Hu[1], and W. A. Curtin[1]**

[1] Laboratory for Multiscale Mechanics Modeling, EPFL, Lausanne, Switzerland
abhinav.jain@epfl.ch, daniel.marchand@epfl.ch, yi.hu@epfl.ch, william.curtin@epfl.ch

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Industrial processing and application of advanced materials requires exquisite control of both composition and processing path to achieve optimal performance. Bridging the chasm between chemical interactions and macroscopic material behavior can be aided by emerging integrated multiscale materials modelling approaches. Here, we illustrate progress in the domain of metallurgy, presenting a multiscale pathway from first-principles modelling to alloy evolution during processing to alloy yield strength for Al-Mg-Si Al-6xxx alloy. A first-principles database of many metallurgically-relevant structures is created and used to develop a Neural Network interatomic potential (NNP) for the Al-Mg-Si system [1]. The NNP is then used in a Kinetic Monte Carlo study of natural aging to demonstrates that early-stage clusters trap vacancies and delay further evolution at room temperature. The NNP is then further used to compute the Generalized Stacking Fault Energy surfaces for the various β" precipitates formed at peak aging [1], and direct atomistic simulations at experimental scales show the shearing and Orowan looping that control alloy strength [2]. Finally, a mesoscale discrete dislocation dynamics method is calibrated to atomistic NNP quantities and used to simulate Orowan looping in realistic 3d precipitate microstructures [2]. While a seamless multiscale path is not yet complete, our progress to date shows how new machine learning potentials provide a crucial quantitative connection between quantum and meso scales.

## REFERENCES

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