# Towards a data-driven multiscale framework for quantum-mechanical investigation of elastic properties of Al-Mg-Zr alloys

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The unique properties of aluminum-based alloys, such as low density, high specific strength, and excellent resistance to oxidation and corrosion, enable the design of advanced metamaterials with applications across aerospace, automotive and structural engineering [1]. In this work, we theoretically investigate the effect of alloying aluminum with magnesium and zirconium on its thermodynamic and mechanical properties. Since exploring the vast chemical compound space of these alloys through Density Functional Theory (DFT) calculations is computationally prohibitive, we developed a scalable and transferable machine learning interatomic potential (MLIP) capable of accurately calculating diverse properties of Al-Mg-Zr alloys, see Figure 1. The MLIP was trained using an active learning technique based on ab initio molecular dynamics simulations, Bayesian statistics, and kernel ridge regression [2]. This methodology ensures that the MLIP captures the effects of alloying concentration and atomic configurations up to the solubility limit, providing access to highly accurate physicochemical properties of wide range of Al-bases alloys at a reasonable computational cost. In addition, we present a detailed analysis of the elastic properties of different phases in the Al-Mg-Zr system. These calculations enable insights into phase-dependent mechanical behavior and their contributions to macroscopic performance, which is of importance for engineering application on the mesoscale and beyond. For instance, the elastic modulus of the $Al_3Zr$ phase is more than double that of the pure aluminum phase, highlighting its potential to significantly enhance the stiffness of the alloy [3]. To further explore the implications of alloying and microstructural design, we simulate the macroscopic response of spinodoid structures using computational continuum mechanics. This approach allows us to analyze the interactions between local elastic heterogeneities and global stress-strain behavior, offering a comprehensive understanding of how alloying and microstructural evolution influence the elastic properties of these materials [4]. By combining MLIP, phase-specific elastic property predictions with quantum-mechanical accuracy and mesoscale continuum modeling, this study establishes a multi-scale framework for investigating and designing advanced aluminum-based alloys with optimized elastic and thermomechanical properties.

## References

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## Figures

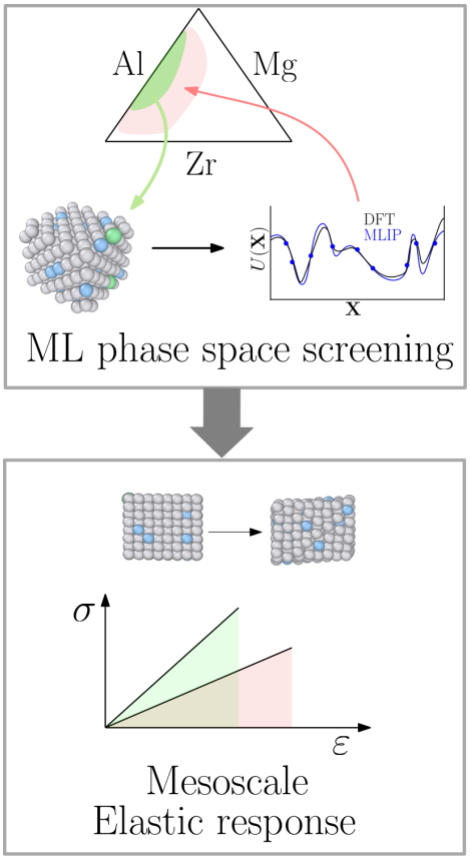


**Figure 1.** Sketch of the workflow. For the relevant phase space in the Al-Mg-Zr ternary phase diagram, MLIP are trained via Bayesian regression. The training includes strained structures, different phases and different concentrations. The resulting MLIPs are applied to the whole relevant phase space up to the solubility limit. From the MLIP/DFT- elastic constants, mesoscale modeling is initiated.