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Accelerated Construction of Equations of States for Elemental and Binary Alloys via Physics-Informed Message Passing Neural Networks

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The current paradigm of discovering, designing and optimising new materials from first-principles simulation can be prohibitively expensive to simulate. Despite the growth in popularity of machine learning to accelerate first principles design and optimisation of materials, data scarcity (Experimental and/or simulated) still poses a challenge. In this study, Physics-Informed Message Passing Neural Network (PI-MPNN) architecture is proposed to construct equations of state from sparse data obtained through Materials project and DFT calculation for elemental and binary metal alloys. The performance of this is compared to traditional MPNN and other machine learning algorithms such as Random Forest, Gradient Boost and regression at 0-15% noise level.

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None

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