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Machine-Learning based potential for Iron: plasticity and phase transition. JEAN-BERNARD MAILLET, CHRISTOPHE DENOUAL, CEA, DAM, DIF, GABOR CSANYI, Engineering Laboratory, University of Cambridge — A classical interatomic potential is trained within the GAP framework with the goal of reproducing both plastic properties and phase transition for Iron. We first build a reference compact database based on tight-binding calculations of the magnetic bcc and non magnetic hcp phase, as well as the transition path between the two structures. We then show how the GAP formalism enables the reproduction of complex properties that include equation of state, elasticity, plasticity, and phase transition for this complex system.

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