



Combining phonon accuracy with high transferability in machine-learned interatomic potentials

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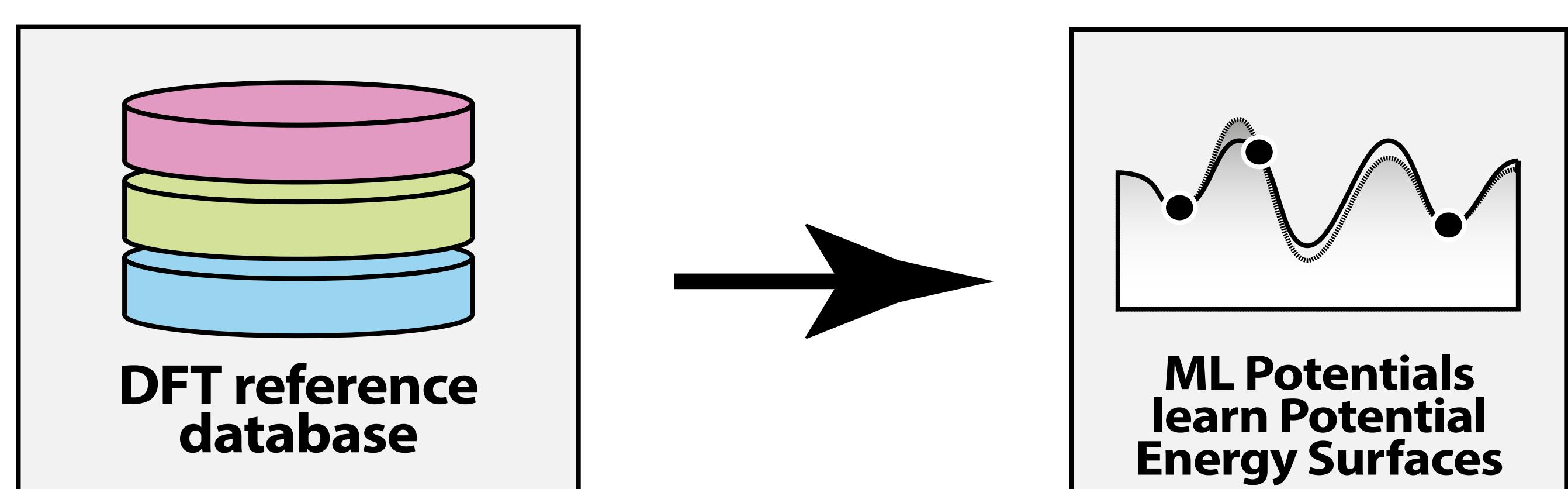
Animated Version



Can we accelerate the prediction of phonon properties with machine-learned interatomic potentials?

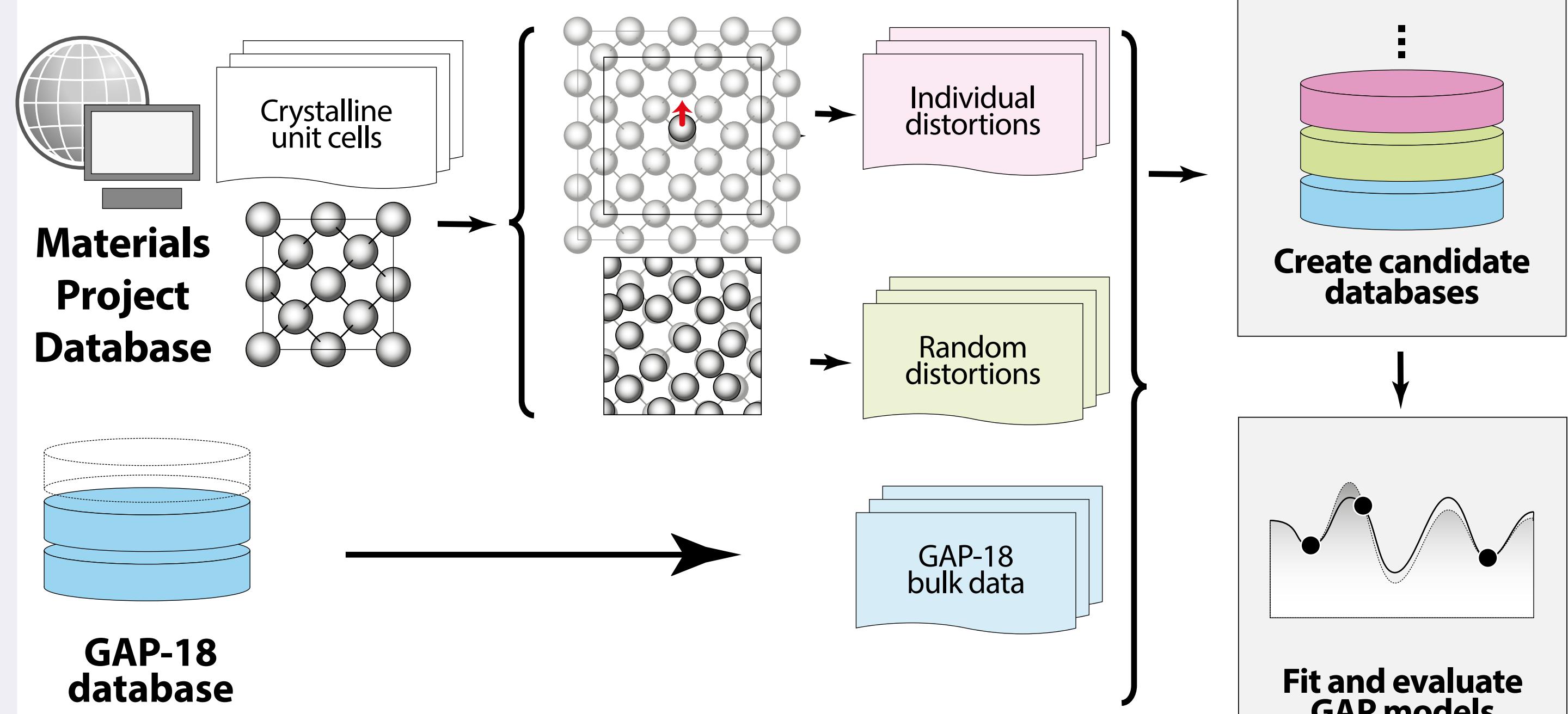
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Idea behind machine-learned interatomic potentials

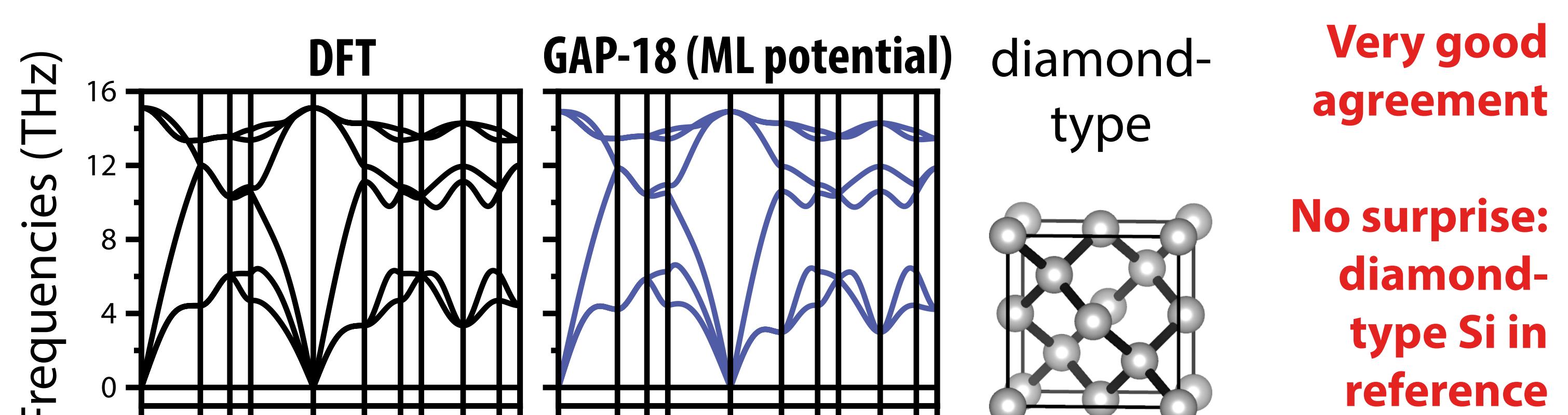


Machine-learned interatomic potentials learn based on reference data (e.g., from density functional theory)

New schemes to build reference databases: more diverse set of structures

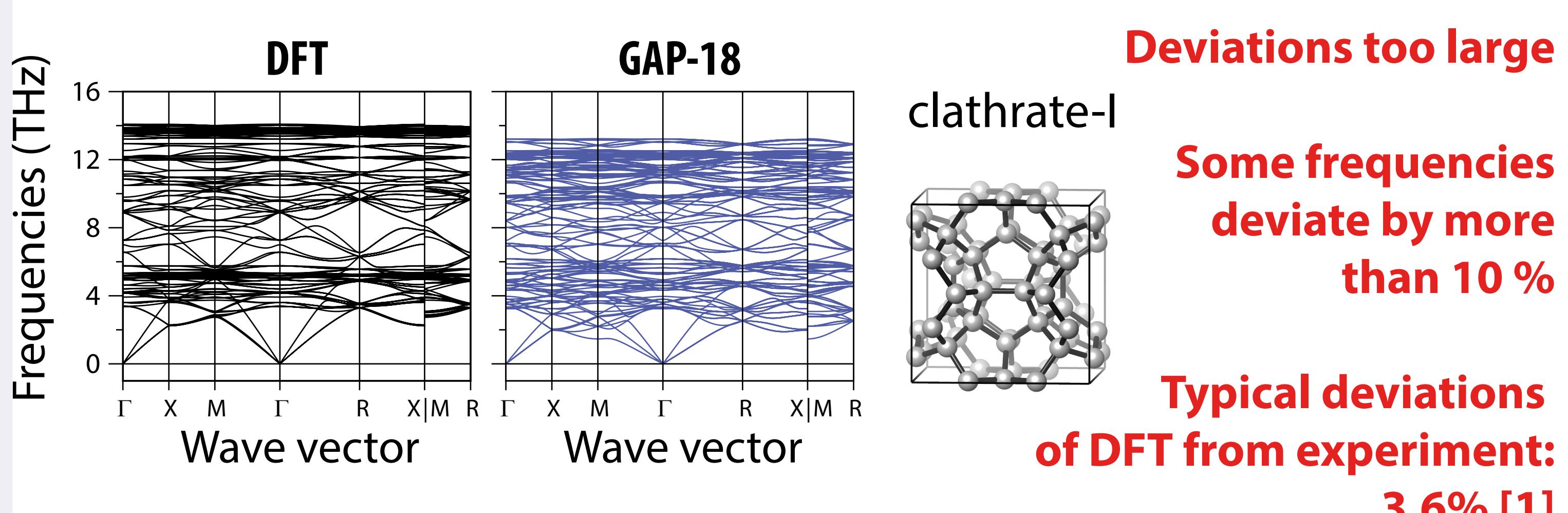


Results of state-of-the-art potential (GAP-18) for phonon properties of Si allotropes



GAP-18: A. P. Bartók, J. Kermode, N. Bernstein, and G. Csányi Phys. Rev. X 2018, 8, 04104

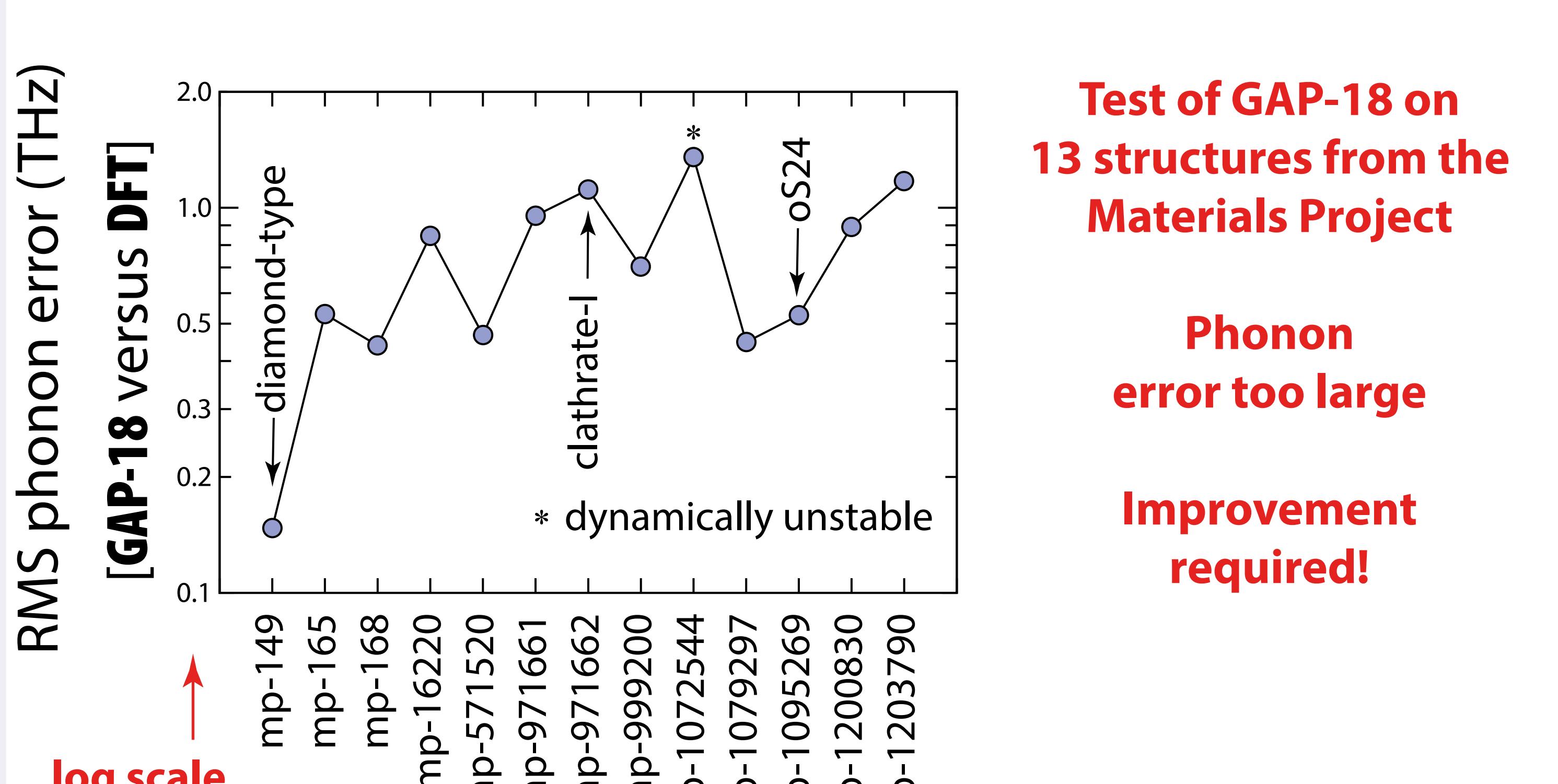
Results of state-of-the-art potential (GAP-18) for phonon properties of Si allotropes



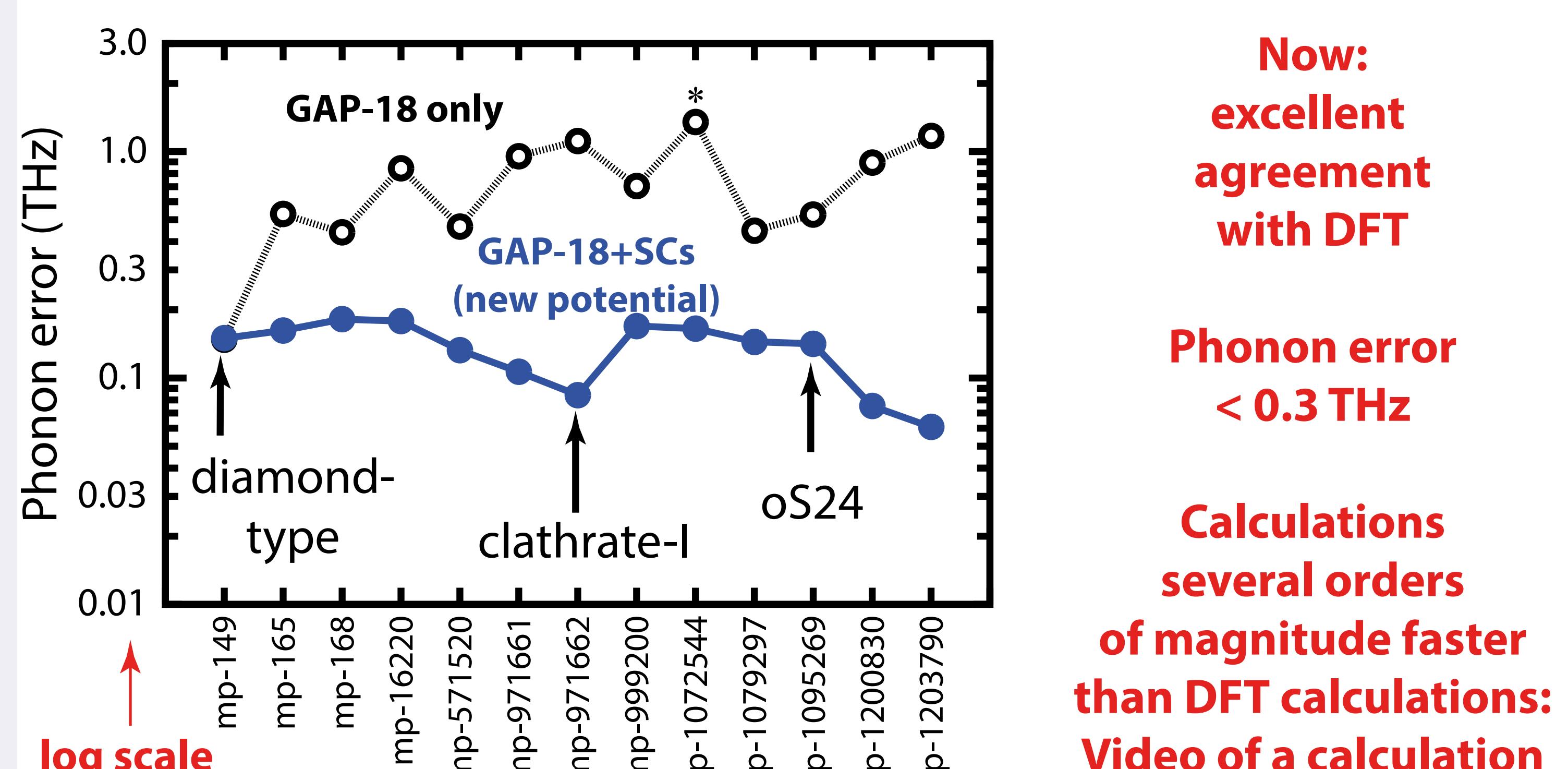
[1] G. Petretto, Scientific Data, 2018, 5, 180065.

GAP-18: A. P. Bartók, J. Kermode, N. Bernstein, and G. Csányi Phys. Rev. X 2018, 8, 04104

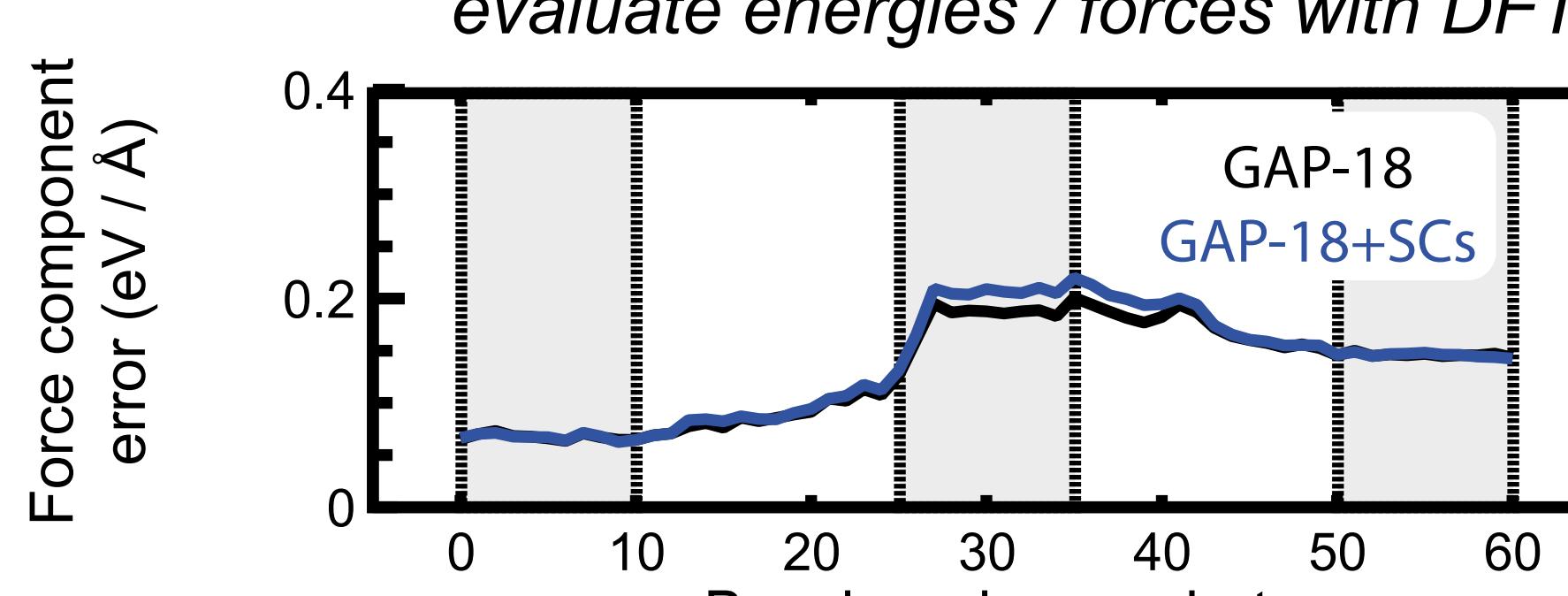
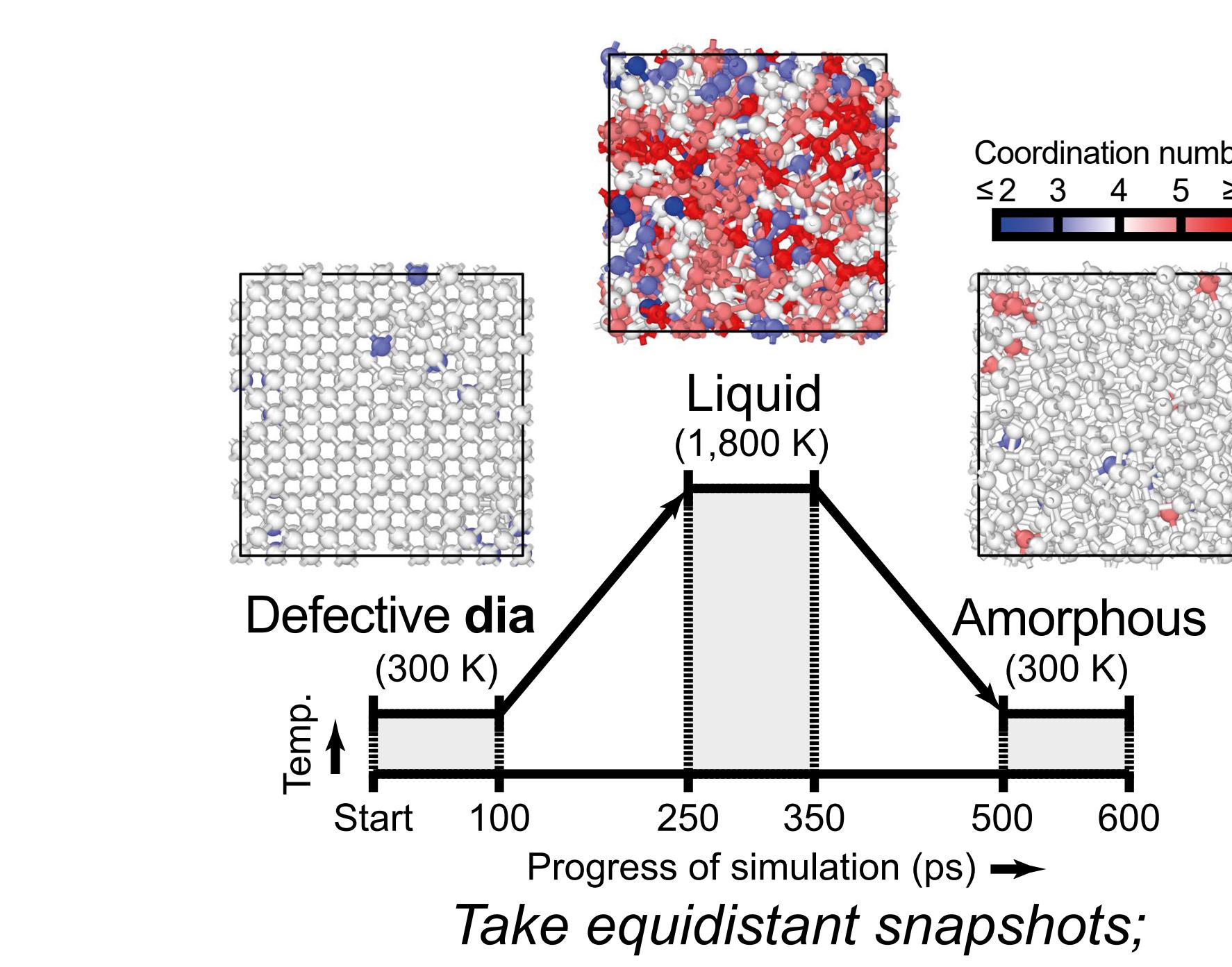
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New Machine-Learned Interatomic Potential: Excellent Prediction of Phonon Properties



New Machine-Learned Interatomic Potential: Melting of defective Silicon



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