

Supplementary Information: Machine-Learned Interatomic Potentials for Alloys

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Supplementary phonon dispersion curve plots for the machine-learned potentials discussed in the main paper.

I. SUPPLEMENTARY NOTES

This section presents phonon dispersion curves for 65 enumerated FCC superstructures with cell sizes from 2 through 6. Special paths in k -space were calculated using the seekpath [1, 2] package. Integrated RMS error is displayed in parentheses next to each potential in the

legend. It is calculated using all eigenvalues at each k -point on a $13 \times 13 \times 13$ grid in the Brillouin zone. Configurations that the potentials used during fitting have “Training” in the title. Those configurations for which phonons are predicted have “Prediction” in the title. Of the 65 configurations, 29 were used for fitting and 36 for validation.

[1] Yoyo Hinuma, Giovanni Pizzi, Yu Kumagai, Fumiyasu Oba, and Isao Tanaka. Band structure diagram paths based on crystallography. *Computational Materials Sci-*

ence, 128:140 – 184, 2017.

[2] Atsushi Togo and Isao Tanaka. `{Spglib}`: a software library for crystal symmetry search. *arXiv e-prints*, page arXiv:1808.01590, Aug 2018.

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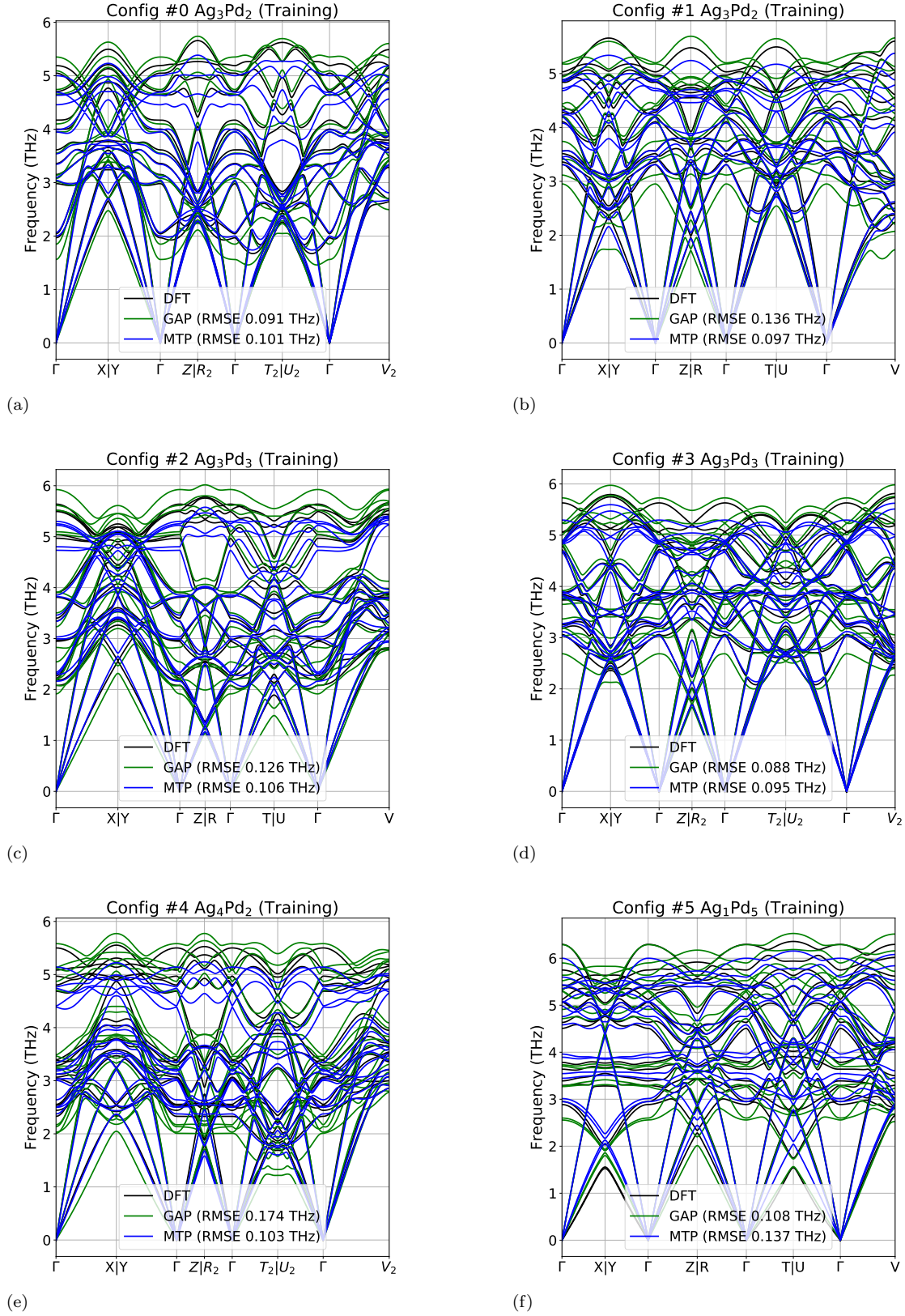


FIG. 1: Phonon predictions for selected configurations.

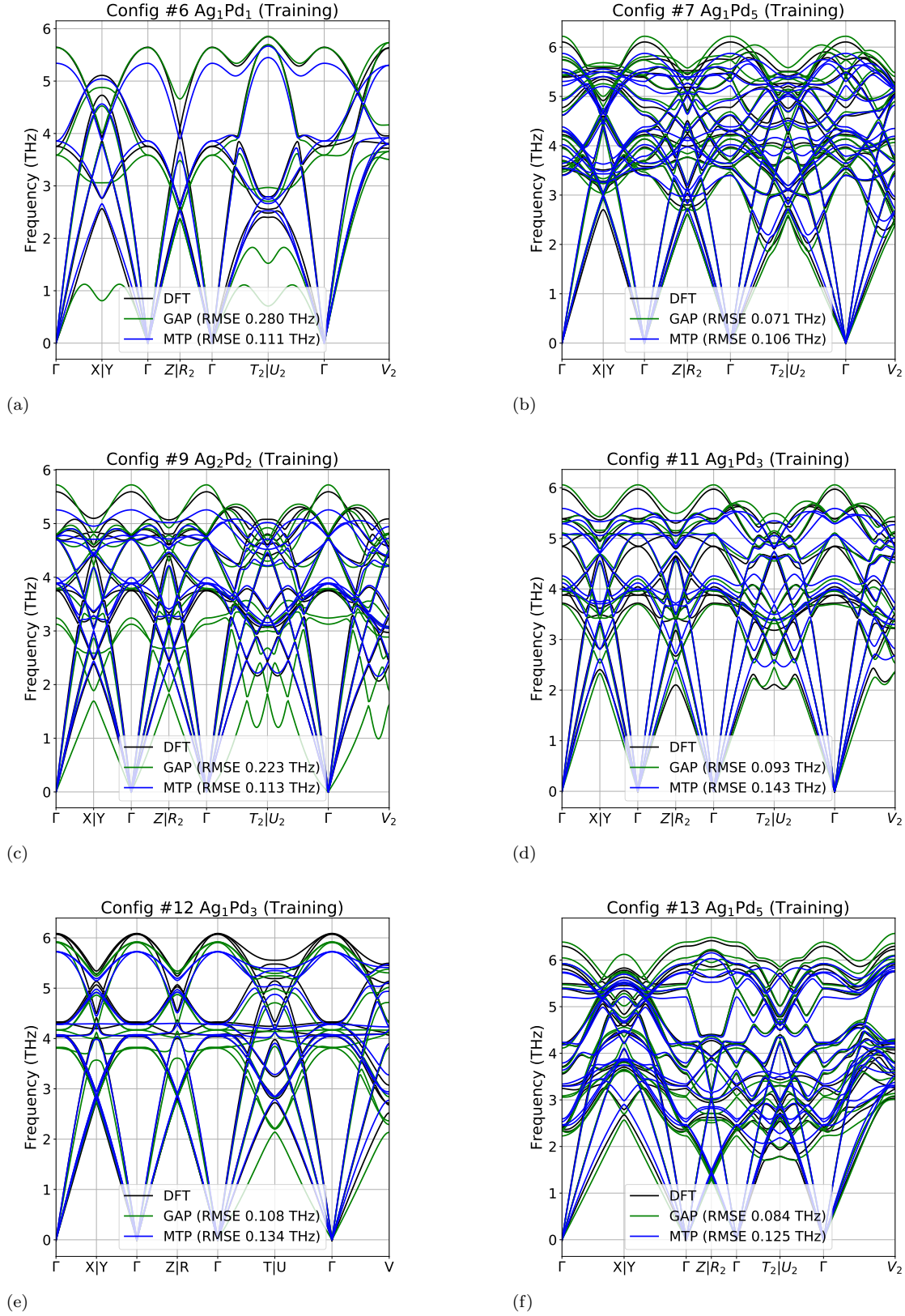


FIG. 2: Phonon predictions for selected configurations.

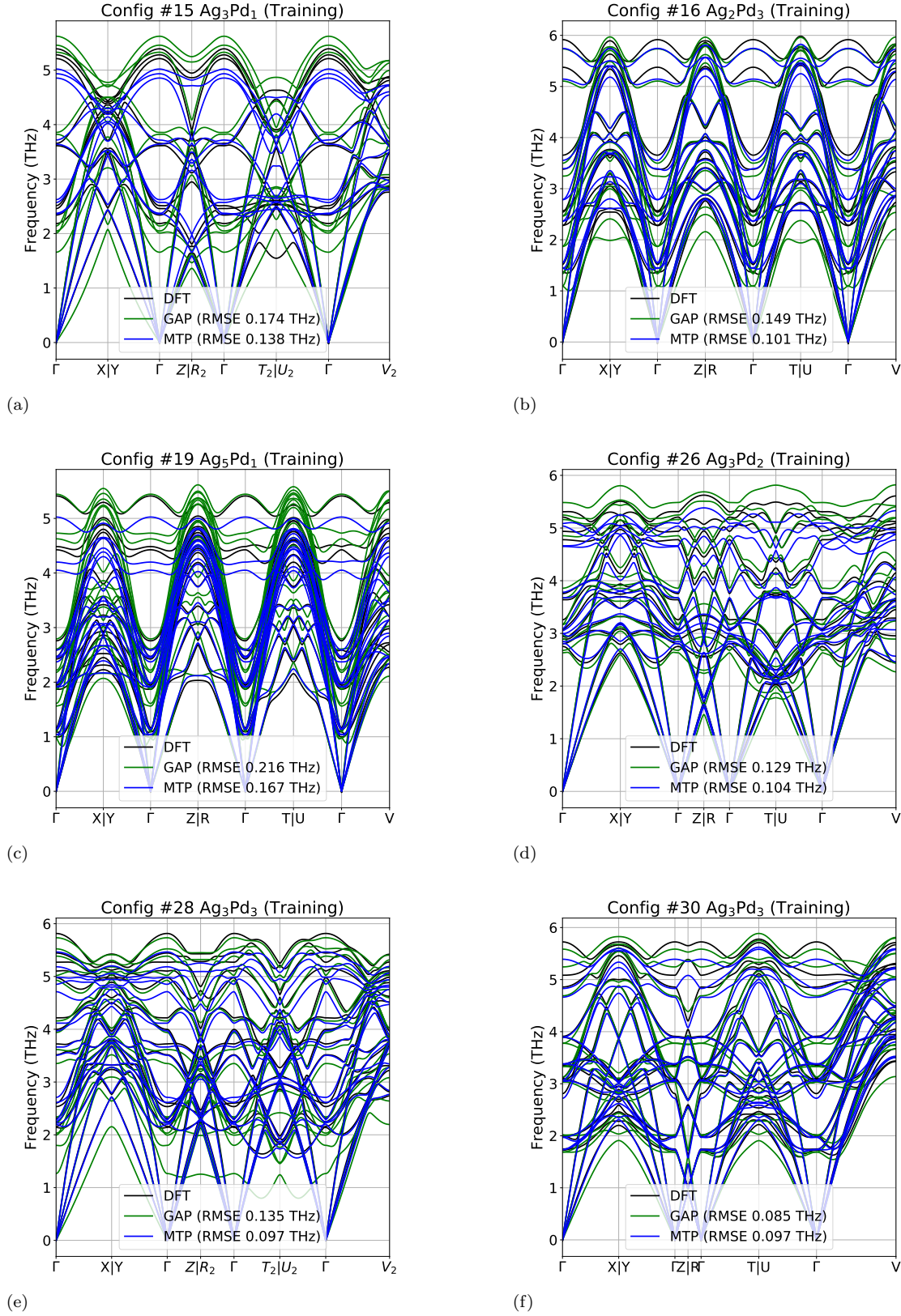


FIG. 3: Phonon predictions for selected configurations.

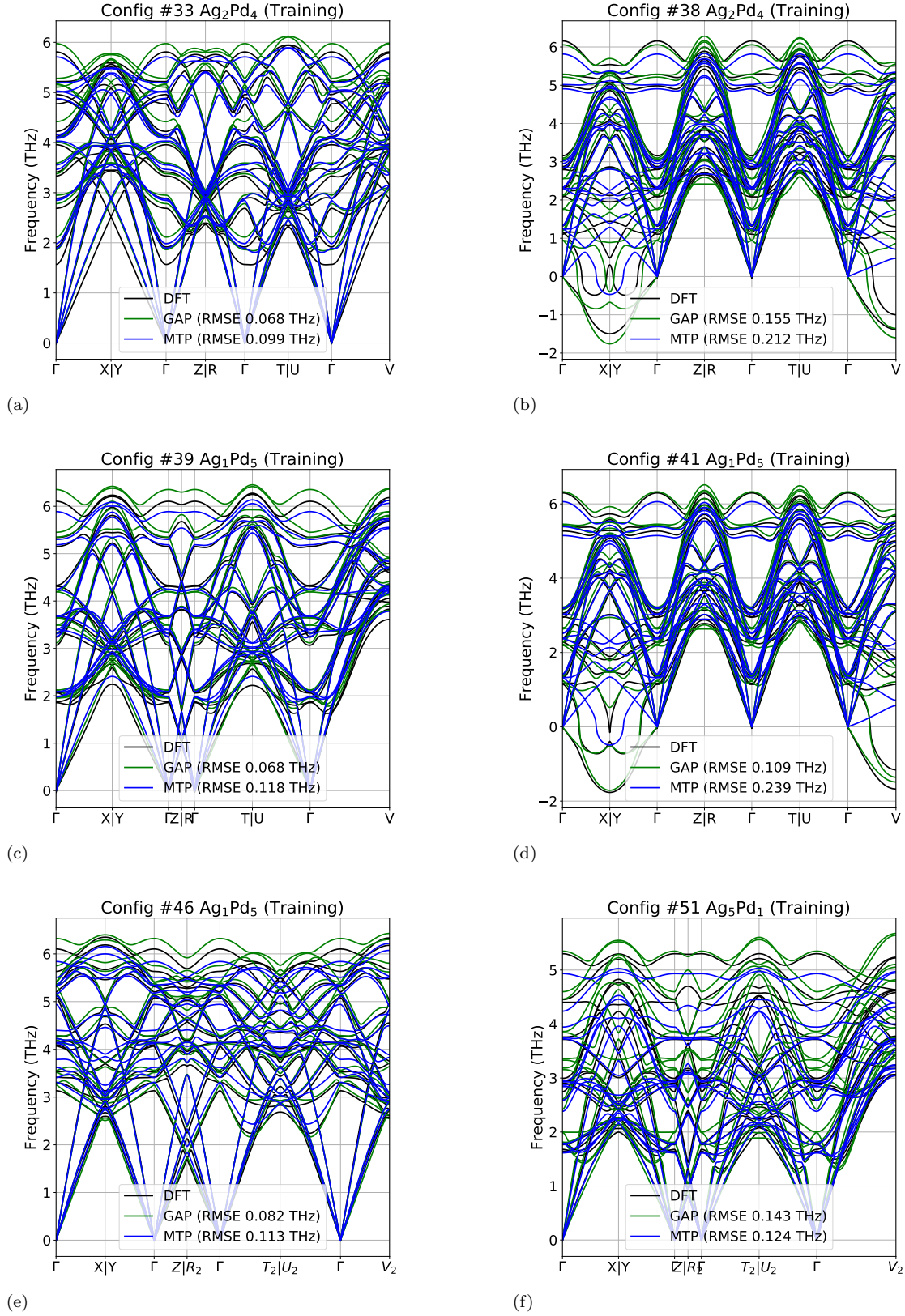
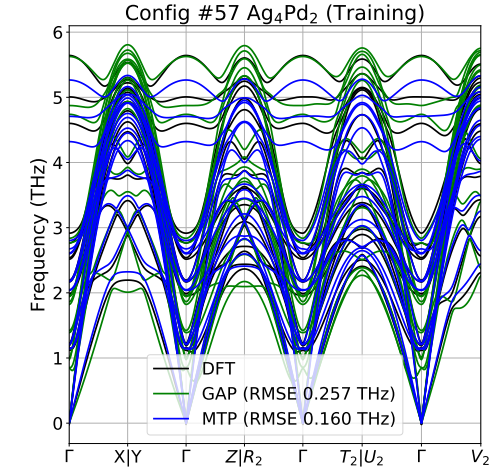
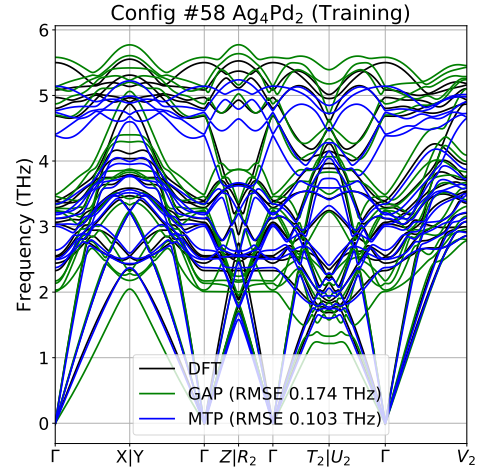


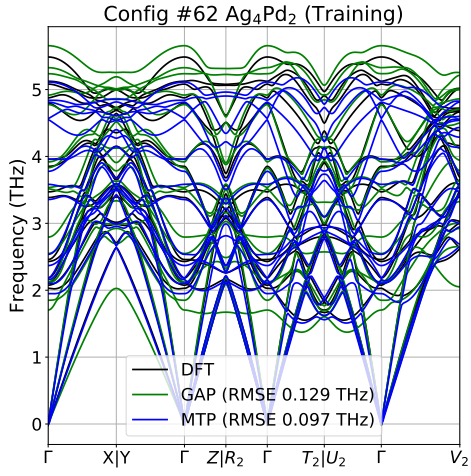
FIG. 4: Phonon predictions for selected configurations.



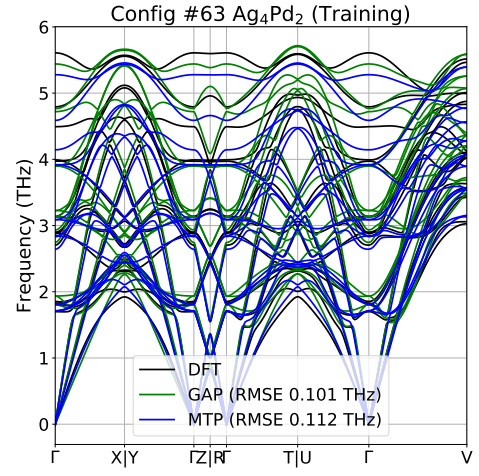
(a)



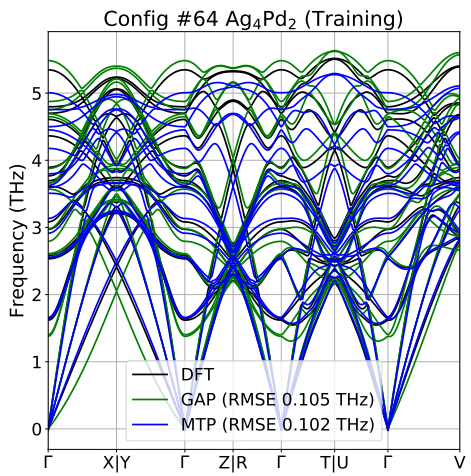
(b)



(c)



(d)



(e)

(f)

FIG. 5: Phonon predictions for selected configurations.

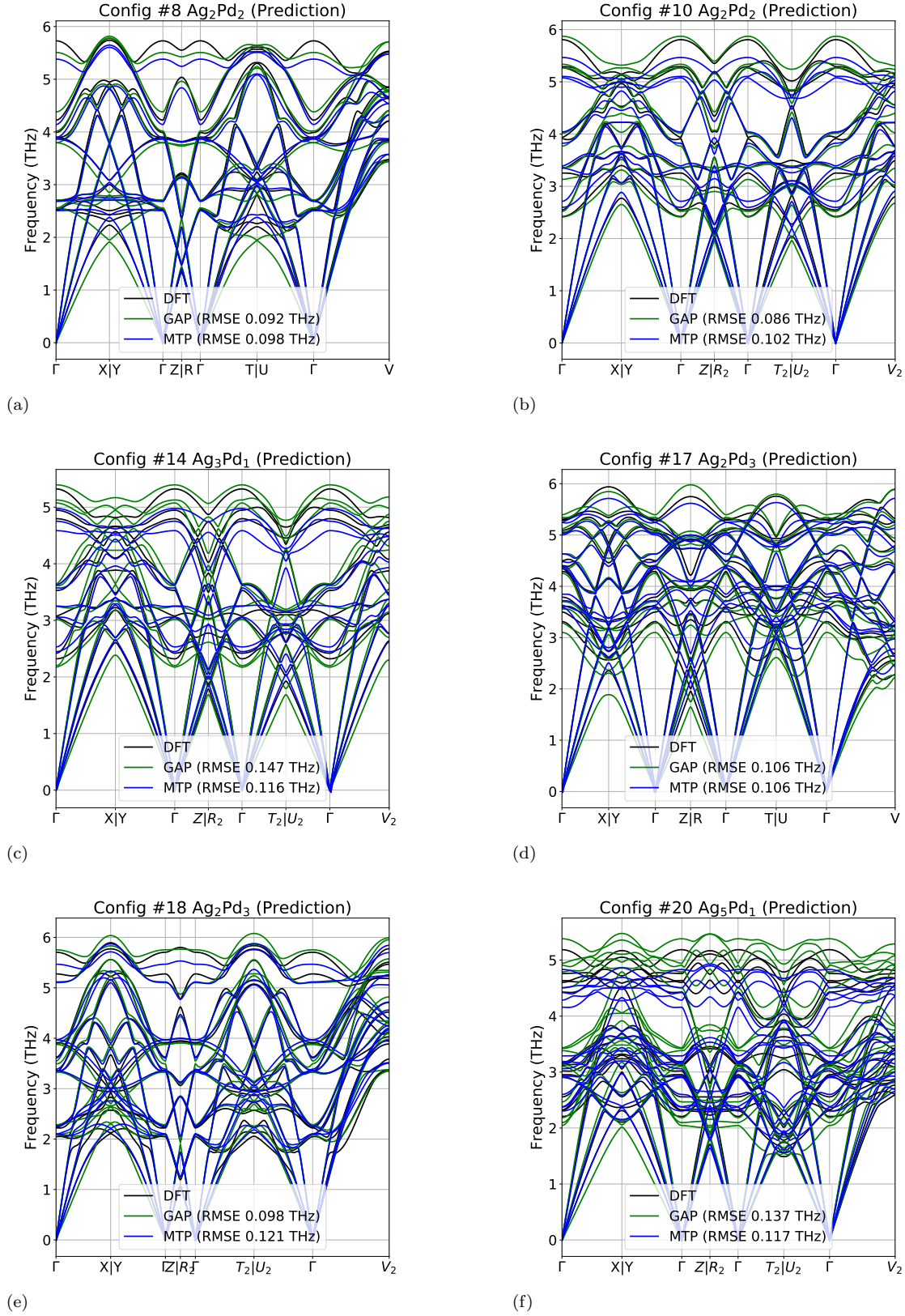


FIG. 6: Phonon predictions for selected configurations.

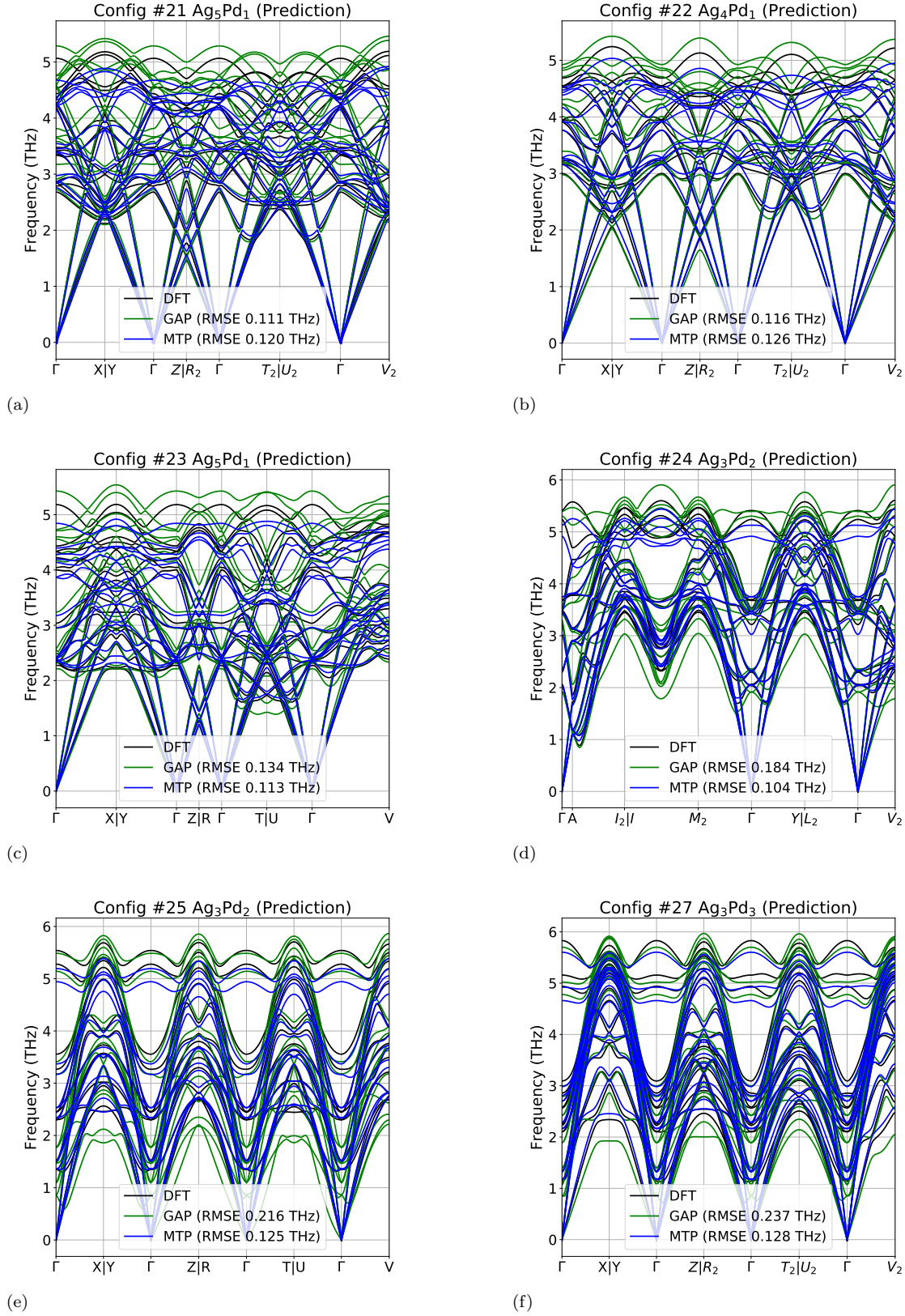


FIG. 7: Phonon predictions for selected configurations.

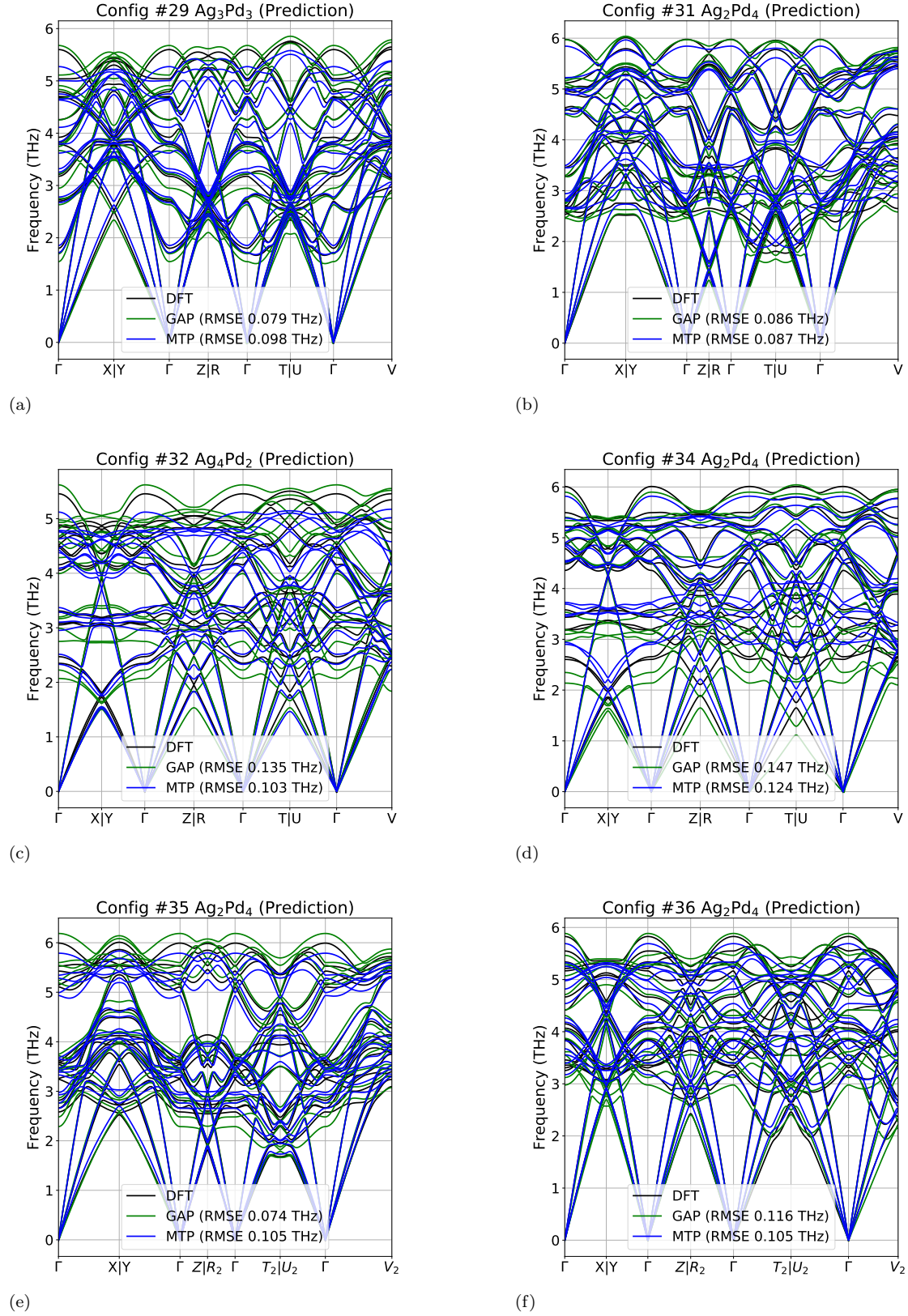


FIG. 8: Phonon predictions for selected configurations.

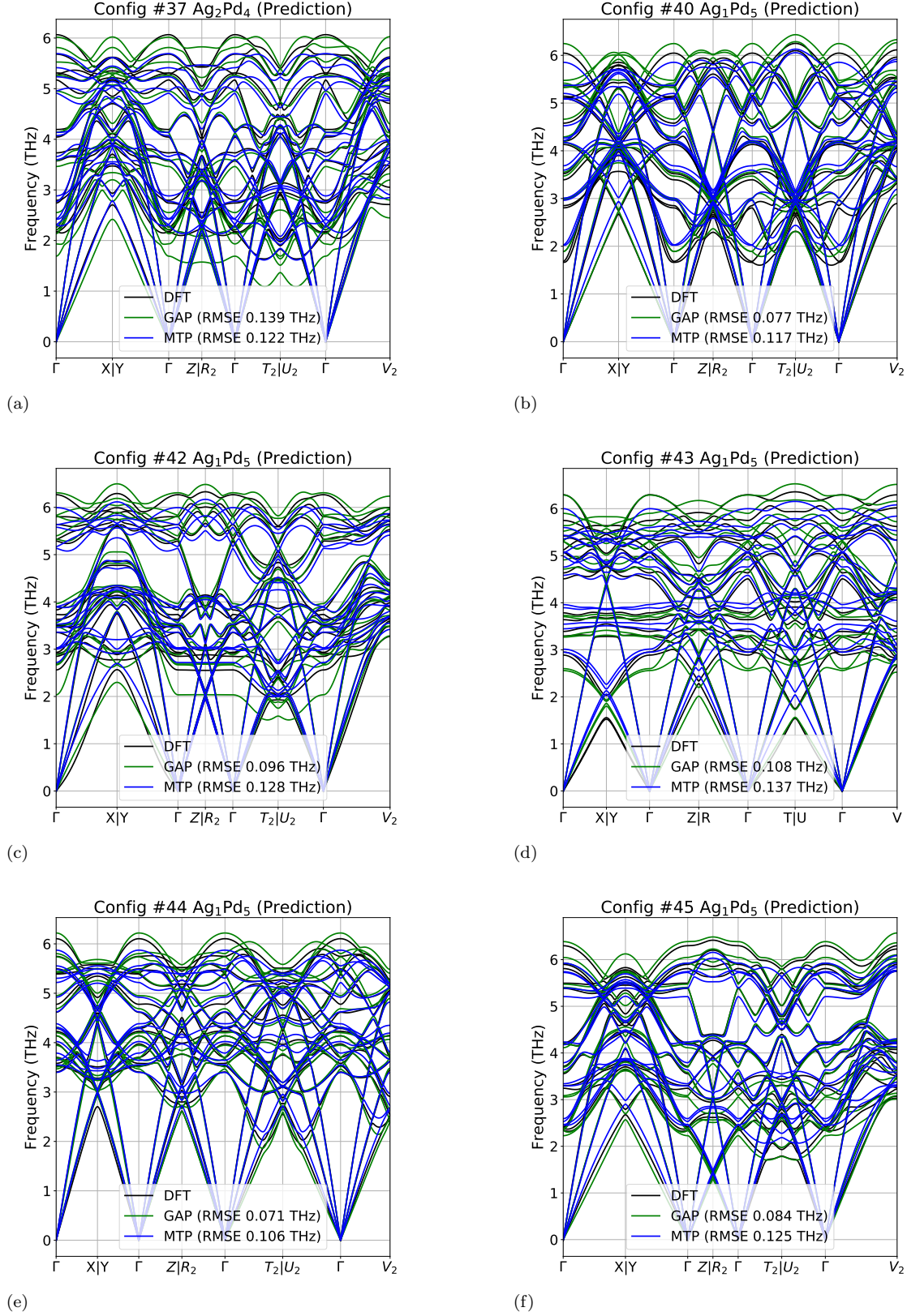


FIG. 9: Phonon predictions for selected configurations.

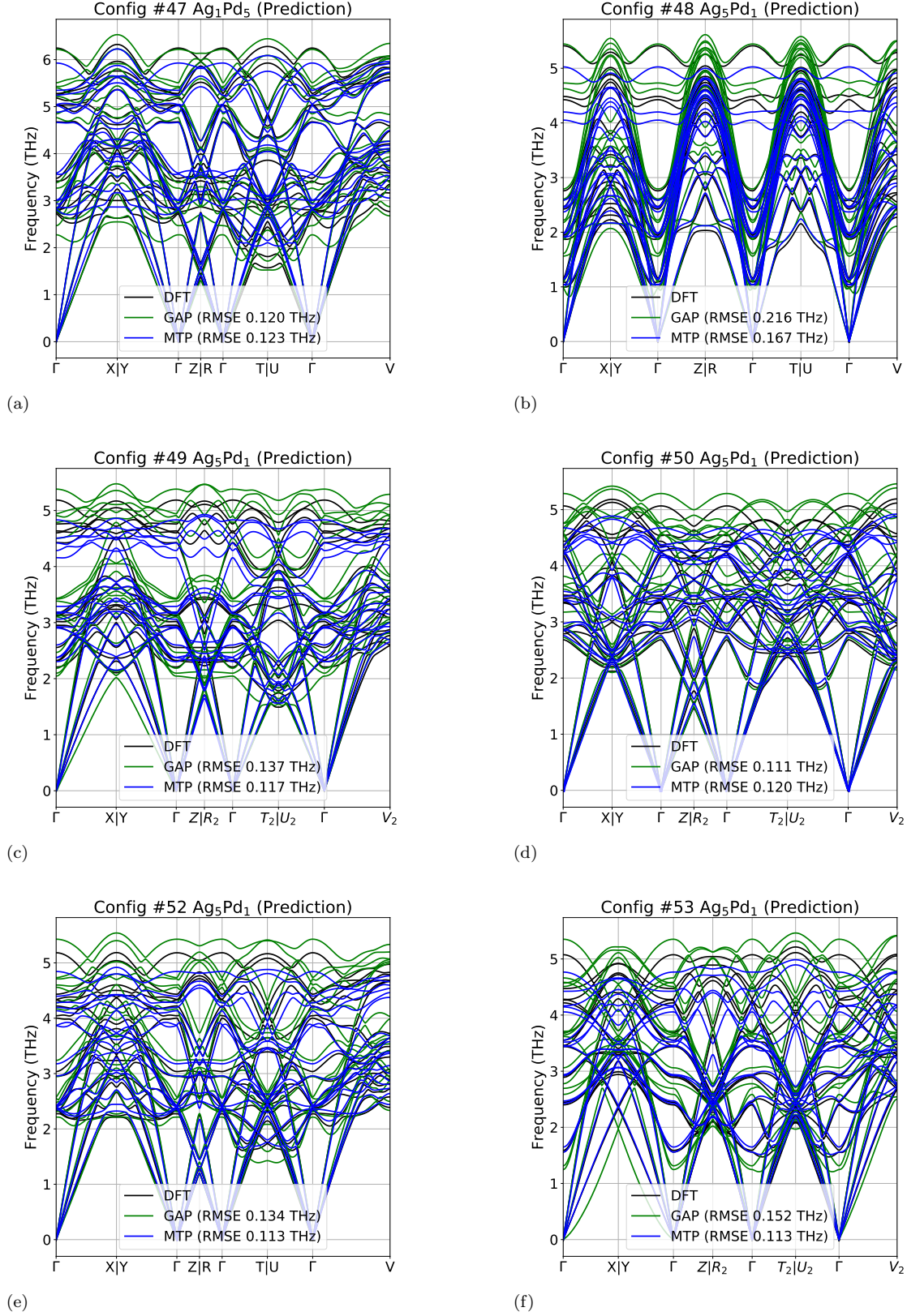


FIG. 10: Phonon predictions for selected configurations.

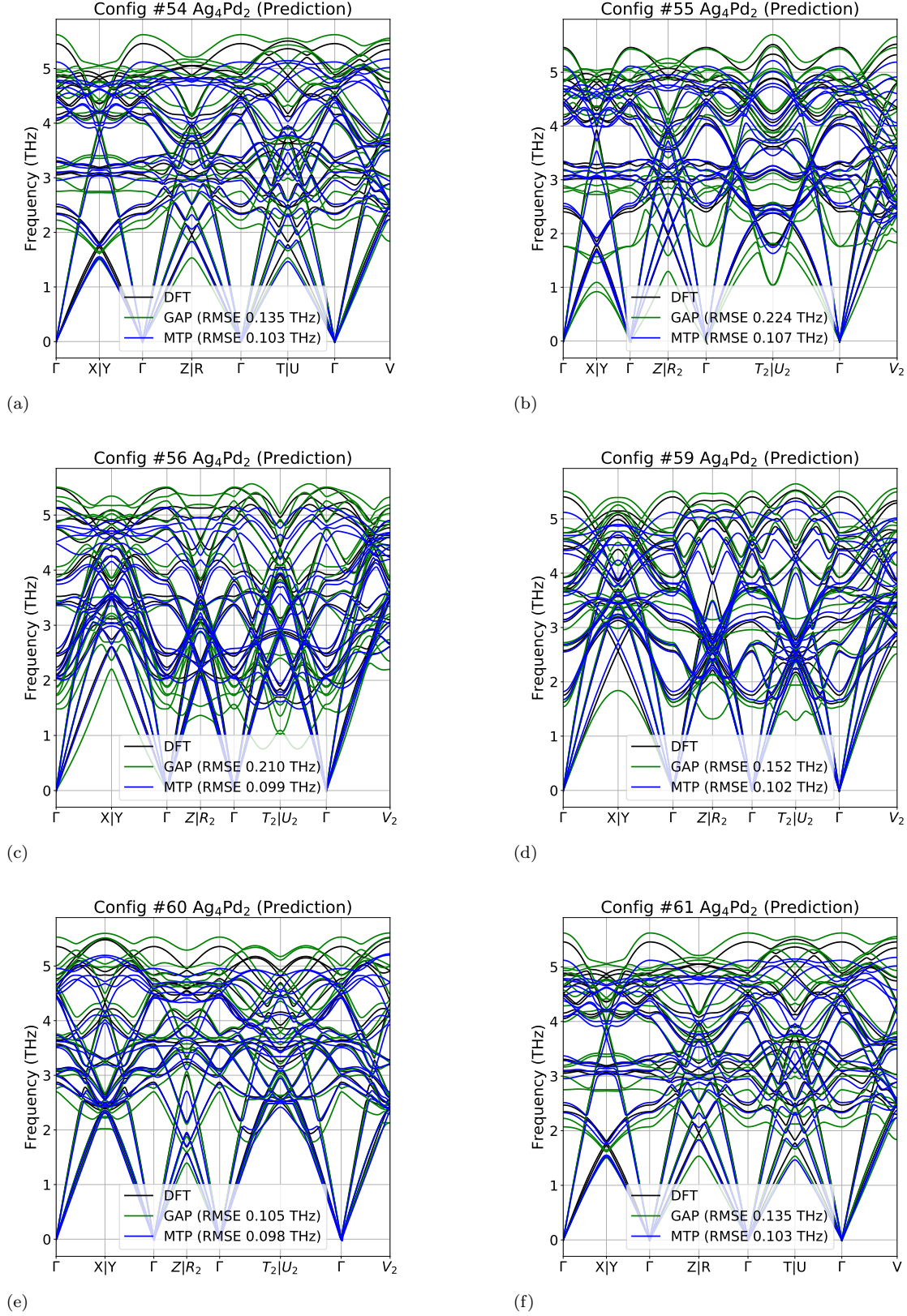


FIG. 11: Phonon predictions for selected configurations.