Accelerating Structure Prediction of Molecular Crystals using Actively Trained Moment Tensor Potential

Supporting Materials

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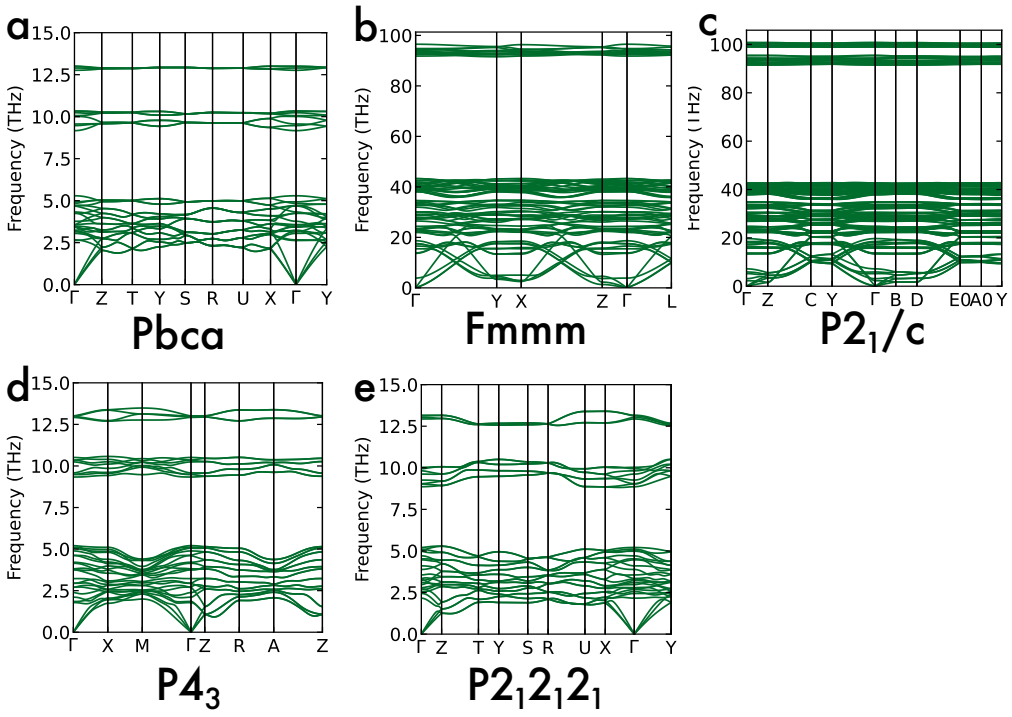

Figure 1: (a-e) Phonon spectrums of various (the most energetically favorable) benzene polymorphs computed using MTP.

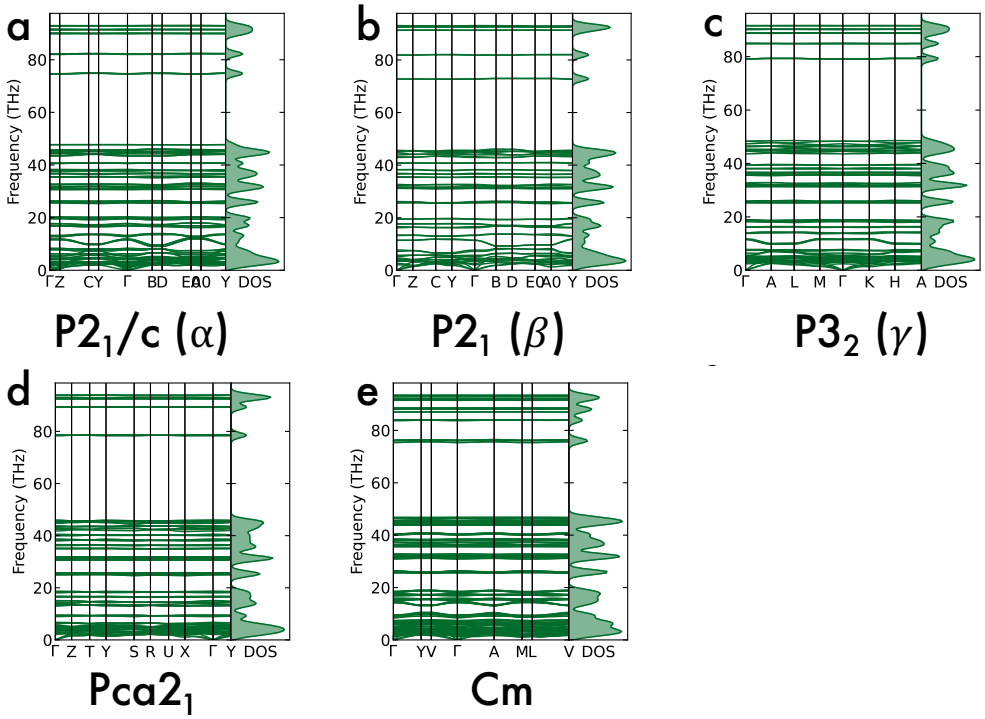

Figure 2: (a-e) Phonon spectrums of various (the most energetically favorable) polymorphs of glycine computed using MTP.