Supplemental Materials: Efficient Modeling of Dynamic Properties in K_3C_{60} Using Machine Learning Force Fields

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S1 ACE radius cutoff

The optimal ACE radius cutoff is determined through scanning for C-C and C-K cutoff radius (Fig. S1). A rough scan of K-K cutoff from 3 to 10 $\mathring{A}$ sees no difference in the resultant likelihood, and is thus arbitrarily set as 5.0 $\mathring{A}$.

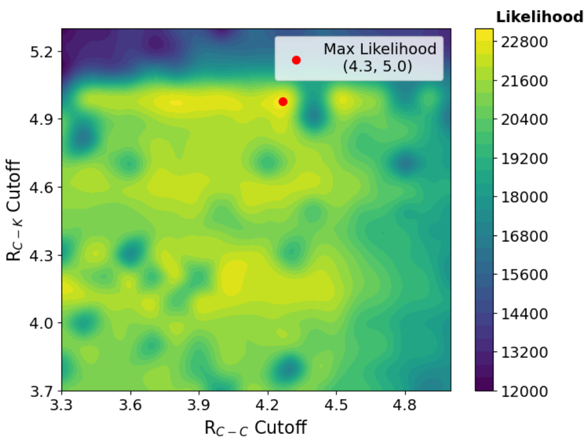

Fig. S1 The likelihood surface for finding optimal radius cutoff of ACE descriptors.

	QE	VASP
DFT	$\begin{pmatrix} 364.46 & 237.58 & 237.58 & 0.00 & 0.00 & 0.00 \\ 237.58 & 364.46 & 237.58 & 0.00 & 0.00 & 0.00 \\ 237.58 & 237.58 & 364.46 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 131.29 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 131.29 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 131.29 \end{pmatrix}$	$\begin{pmatrix} 124.47 & 266.34 & 266.34 & 0.00 & 0.00 & 0.00 \\ 266.34 & 124.47 & 266.34 & 0.00 & 0.00 & 0.00 \\ 266.34 & 266.34 & 124.47 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 15.21 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 15.21 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 15.21 \end{pmatrix}$
MLFF	$\begin{pmatrix} 76.53 & 39.12 & 39.12 & 0.00 & 0.00 & 0.00 \\ 39.12 & 76.53 & 39.12 & 0.00 & 0.00 & 0.00 \\ 39.12 & 39.12 & 76.53 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 123.12 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 123.12 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 123.12 \end{pmatrix}$	$\begin{pmatrix} 408.11 & 250.88 & 250.88 & 0.00 & 0.00 & 0.00 \\ 250.88 & 408.11 & 250.88 & 0.00 & 0.00 & 0.00 \\ 250.88 & 250.88 & 408.11 & 0.00 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 201.12 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 201.12 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 201.12 \end{pmatrix}$
MD(LJ)	$\begin{pmatrix} 489.41 & 223.00 & 222.51 & 0.73 & 0.25 & -0.67 \\ 223.00 & 489.97 & 222.98 & 0.01 & 0.04 & 0.02 \\ 222.51 & 222.98 & 489.48 & 0.73 & 0.25 & -0.59 \\ 0.73 & 0.01 & 0.73 & 101.01 & -0.73 & -0.01 \\ 0.25 & 0.04 & 0.25 & -0.73 & 101.06 & 0.60 \\ -0.67 & 0.02 & -0.59 & -0.01 & 0.60 & 101.07 \end{pmatrix}$	

Table S1 Elastic tensor from MLFF (VASP, Flare+QE), with comparison to the DFT data (DFT, QE), as well as the molecular dynamic (MD) method with Lennard-Jones (LJ) potential.

S2 Elastic tensor

The Comparison of the elastic tensor matrix is summarized in Table S1

S3 Training Set Crosscheck

A cross-check of the training set is performed. The training data sets calculated by VASP and QE sampled under SOAP and ACE schemes respectively (labeled as VASPset and QEset), are swapped and refitted with the other scheme. The phonon dispersions calculated by the resultant models are compared with that predicted by the model trained by the same data set (S2).

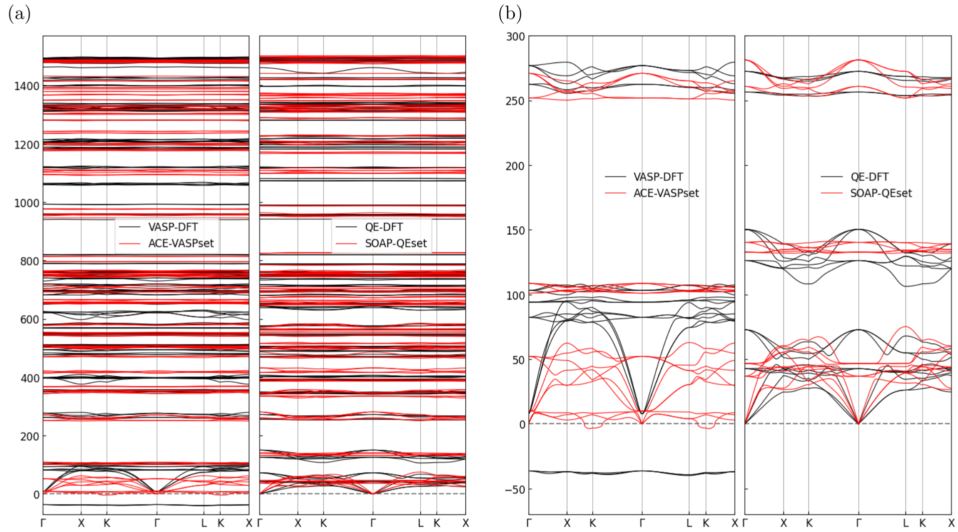

Fig. S2 Comparison of phonon dispersion (cm^{-1}) calculated by models trained with the same DFT data sets on different schemes. (a) full phonon dispersions, (b) phonon dispersion in the low energy region (below 300 cm^{-1})