Electronic Supplementary Material (ESI) for Digital Discovery.

Convergence acceleration with low-precision data in machine learning molecular dynamics

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Table S1. Conversion of linear k-space sampling densities (Δk, top row) to equivalent sampling in both grid notation and k-points per reciprocal atom (pra) in the 1st BZ.

	Δk (Å^{-1})	0.09	0.12	0.18	0.24	0.30	0.36	0.66	0.96
Al	**BCC**	23 x 23 x 23 25000 pra	17 x 17 x 17 9900 pra	11 x 11 x 11 2700 pra	9 x 9 x 9 1500 pra	7 x 7 x 7 700 pra	6 x 6 x 6 500 pra	3 x 3 x 3 100 pra	3 x 3 x 3 100 pra
	FCC	19 x 19 x 19 24000 pra	13 x 13 x 13 8800 pra	9 x 9 x 9 3000 pra	7 x 7 x 7 1400 pra	6 x 6 x 6 900 pra	5 x 5 x 5 500 pra	3 x 3 x 3 200 pra	2 x 2 x 2 100 pra
	HCP	29 x 29 x 15 26000 pra	22 x 22 x 12 12000 pra	15 x 15 x 8 3600 pra	11 x 11 x 6 1500 pra	9 x 9 x 5 900 pra	8 x 8 x 4 600 pra	4 x 4 x 3 100 pra	3 x 3 x 2 50 pra
Cu	**BCC**	25 x 25 x 25 32000 pra	19 x 19 x 19 14000 pra	13 x 13 x 13 4400 pra	10 x 10 x 10 2000 pra	8 x 8 x 8 1100 pra	7 x 7 x 7 700 pra	4 x 4 x 4 200 pra	3 x 3 x 3 100 pra
	FCC	21 x 21 x 21 38000 pra	15 x 15 x 15 14000 pra	10 x 10 x 10 4000 pra	8 x 8 x 8 2100 pra	6 x 6 x 6 900 pra	5 x 5 x 5 500 pra	3 x 3 x 3 200 pra	2 x 2 x 2 100 pra
	HCP	33 x 33 x 17 38000 pra	26 x 26 x 14 19000 pra	17 x 17 x 9 5300 pra	13 x 13 x 7 2400 pra	11 x 11 x6 1500 pra	9 x 9 x 5 900 pra	5 x 5 x 3 200 pra	4 x 4 x 2 100 pra
Mg	**BCC**	21 x 21 x 21 19000 pra	15 x 15 x 15 6800 pra	10 x 10 x 10 2000 pra	8 x 8 x 8 1100 pra	6 x 6 x 6 500 pra	5 x 5 x 5 300 pra	3 x 3 x 3 100 pra	2 x 2 x 2 50 pra
	FCC	17 x 17 x 17 20000 pra	12 x 12 x 12 7000 pra	8 x 8 x 8 2100 pra	6 x 6 x 6 1000 pra	5 x 5 x 5 500 pra	4 x 4 x 4 300 pra	3 x 3 x 3 200 pra	2 x 2 x 2 50 pra
	HCP	31 x 31 x 17 33000 pra	23 x 23 x 13 14000 pra	16 x 16 x 9 4700 pra	12 x 12 x 7 2100 pra	10 x 10 x 5 1000 pra	8 x 8 x 5 700 pra	5 x 5 x 3 200 pra	3 x 3 x 2 50 pra

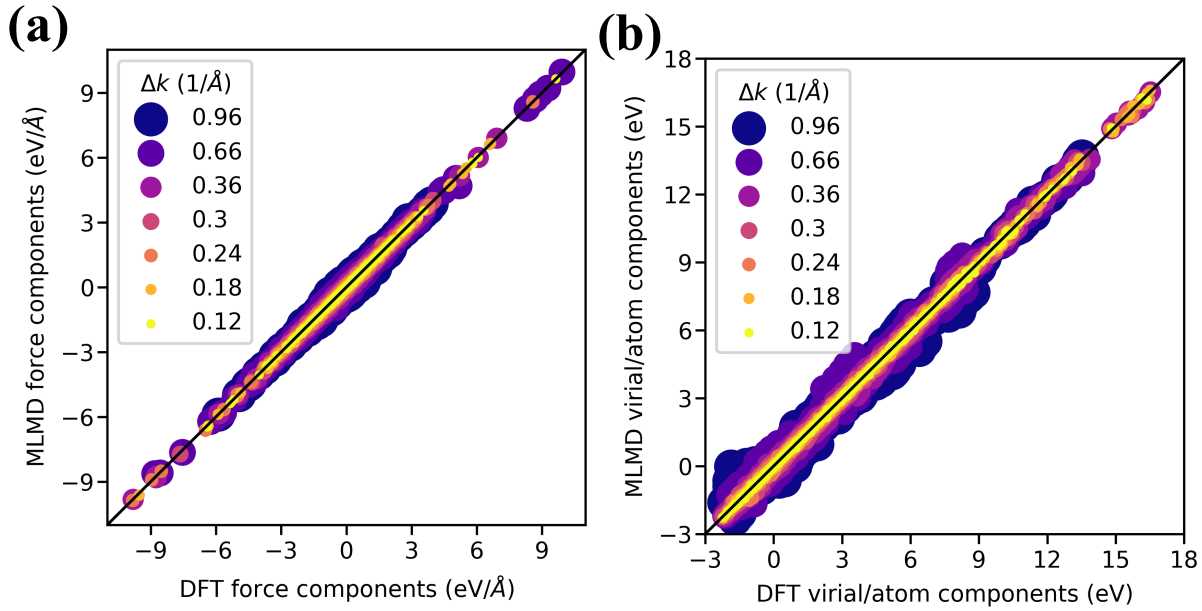

Figure S2. Parity plots of force components (a) and virial components per atom (b) for MLMD models against DFT training data. Legend indicates k-space sampling density (Δk) of the corresponding DFT training dataset.

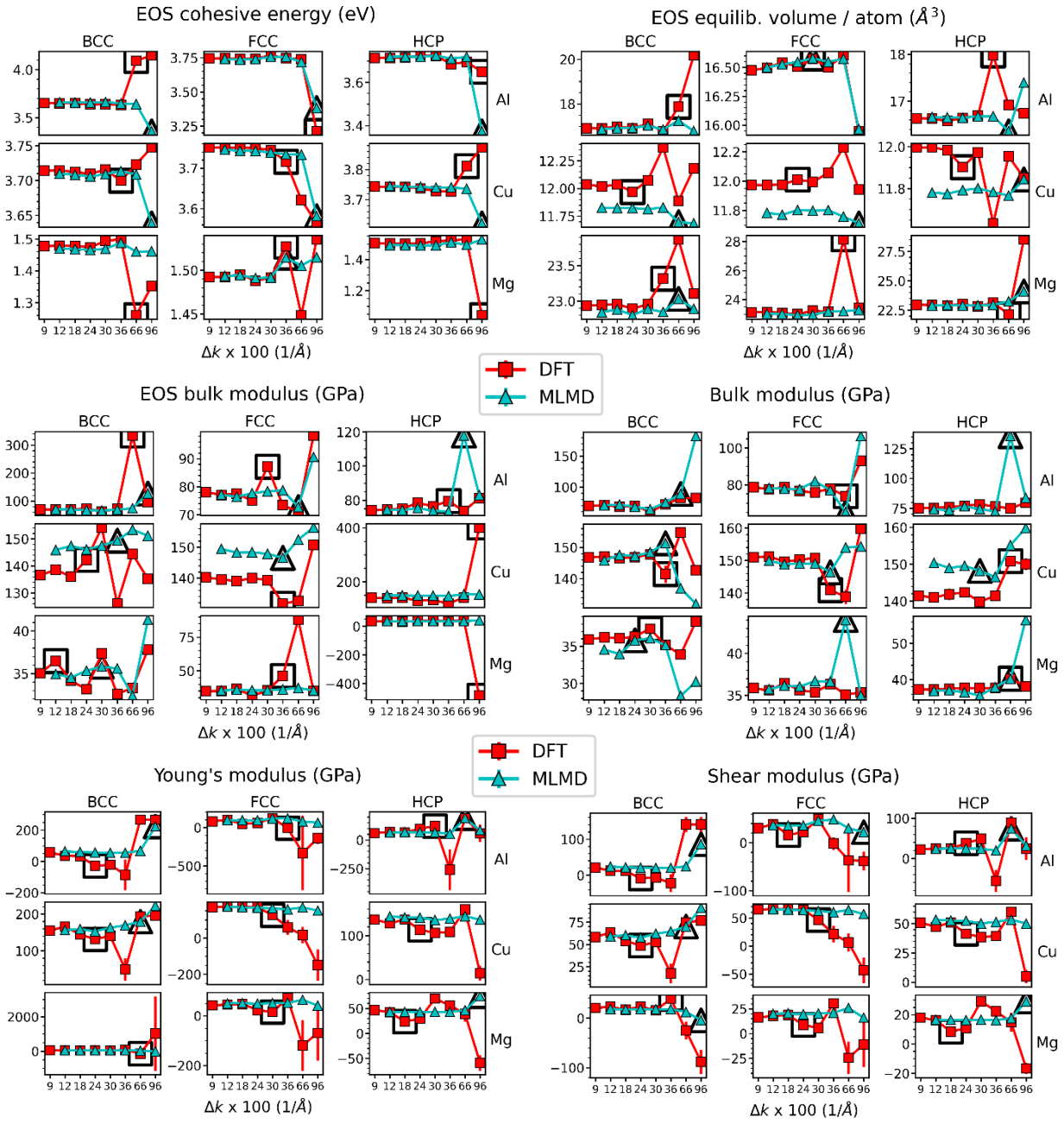

Figure S3. Material properties calculated by both DFT and MLMD plotted as a function of the k-space sampling density parameter Δk. Threshold Δk (Δk_T) where property prediction deviates from that at Δk_{min} by $\frac{1}{2} MAD_{max}$ are highlighted with large black-outlined symbols.

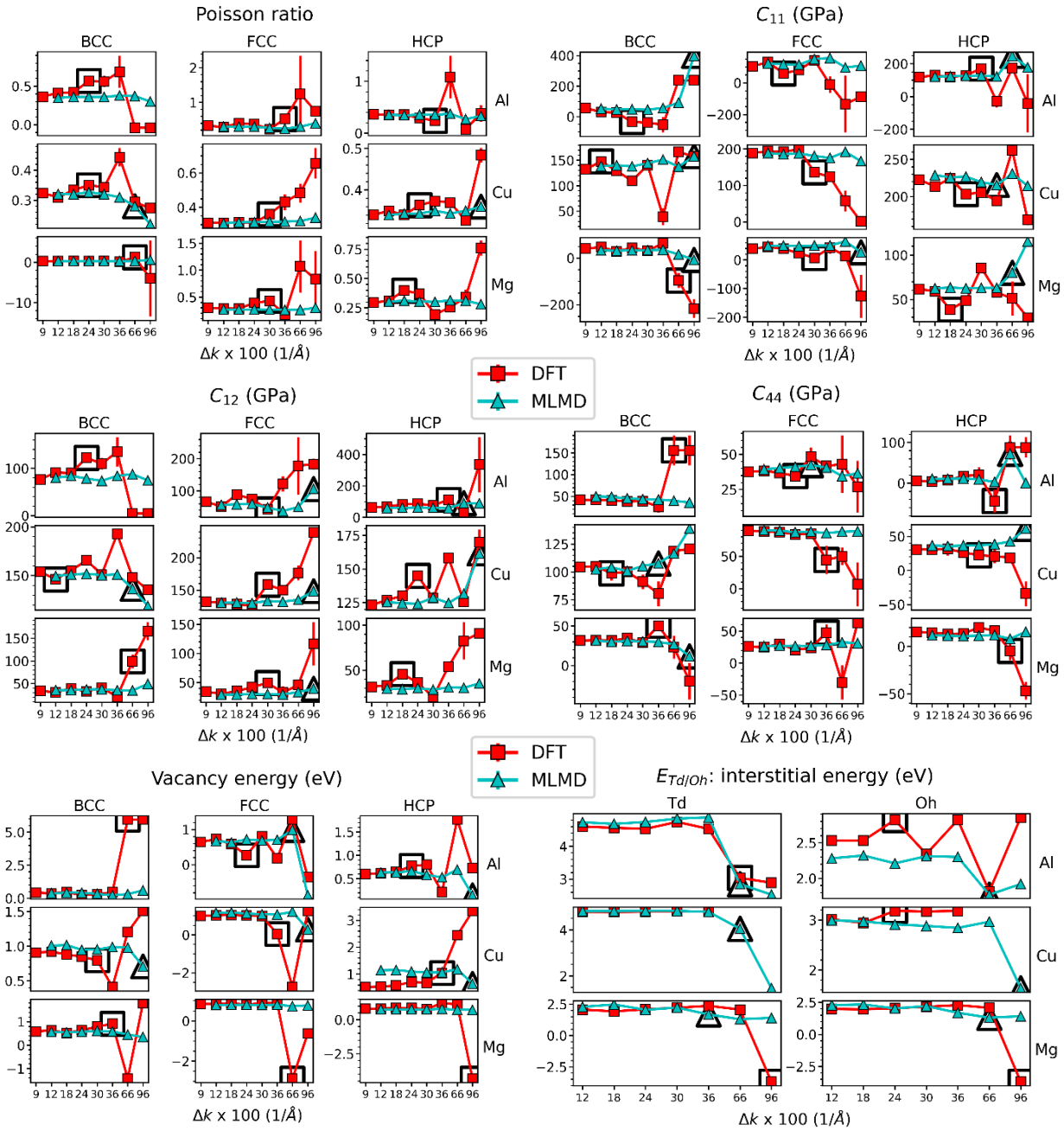

Figure S3 (continued). Additional material properties calculated by both DFT and MLMD plotted versus Δk with Δk_T highlighted by large black-outlined symbols. The interstitial energies were calculated only for equilibrium lattices (FCC-Al, FCC-Cu, HCP-Mg) for each atom type.

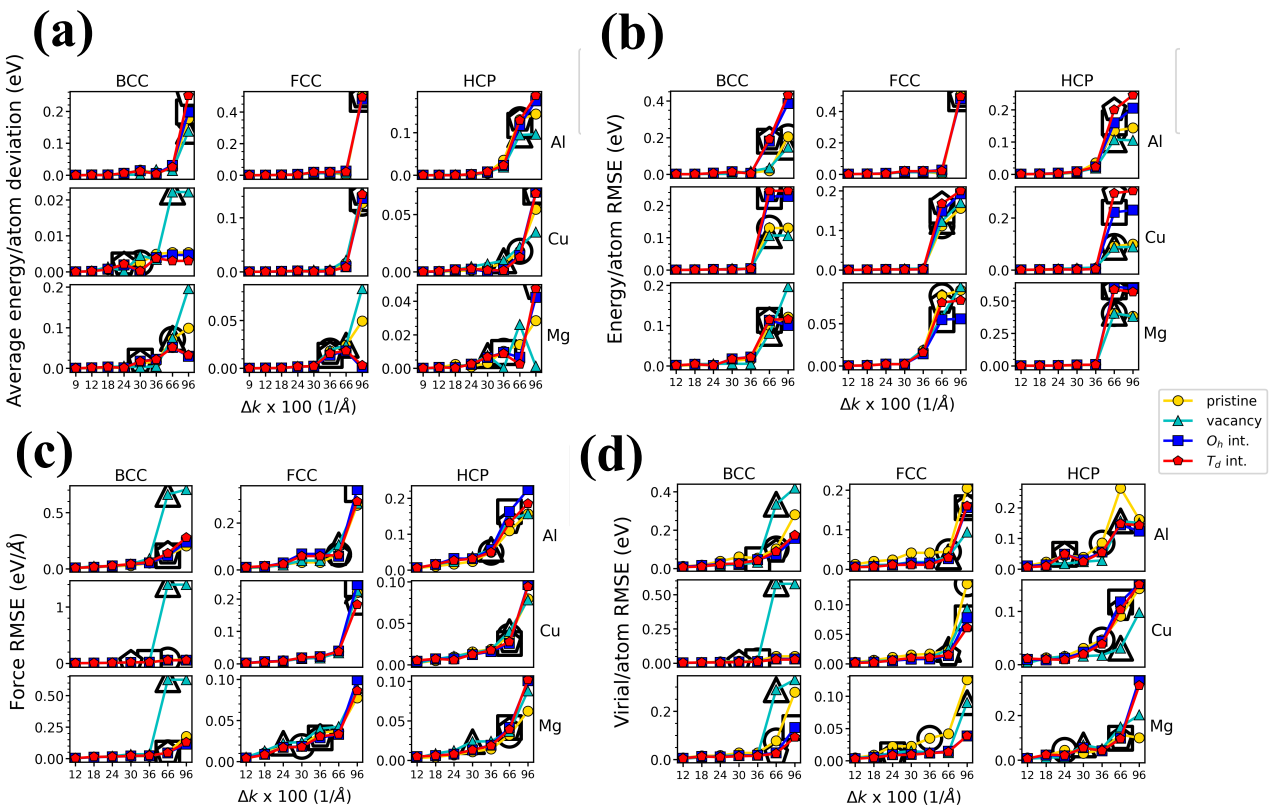

Figure S4. Statistical error metrics (SEMs) of single-point DFT calculations as a function of Δk for the 3600 configurations of the test dataset. The average energy per atom deviation (AEAD) (a), the energy per atom RMSE (E-RMSE) (b), the RMSE of interatomic force components (F-RMSE) (c), and the virial per atom RMSE (V-RMSE) (d). Threshold Δk determined by the $\frac{1}{2} MAD$ criterion is highlighted by large black-outlined symbols.