Supporting Information for:

MS25: Materials Science Focused Benchmark Dataset for Machine Learning Interatomic Potentials

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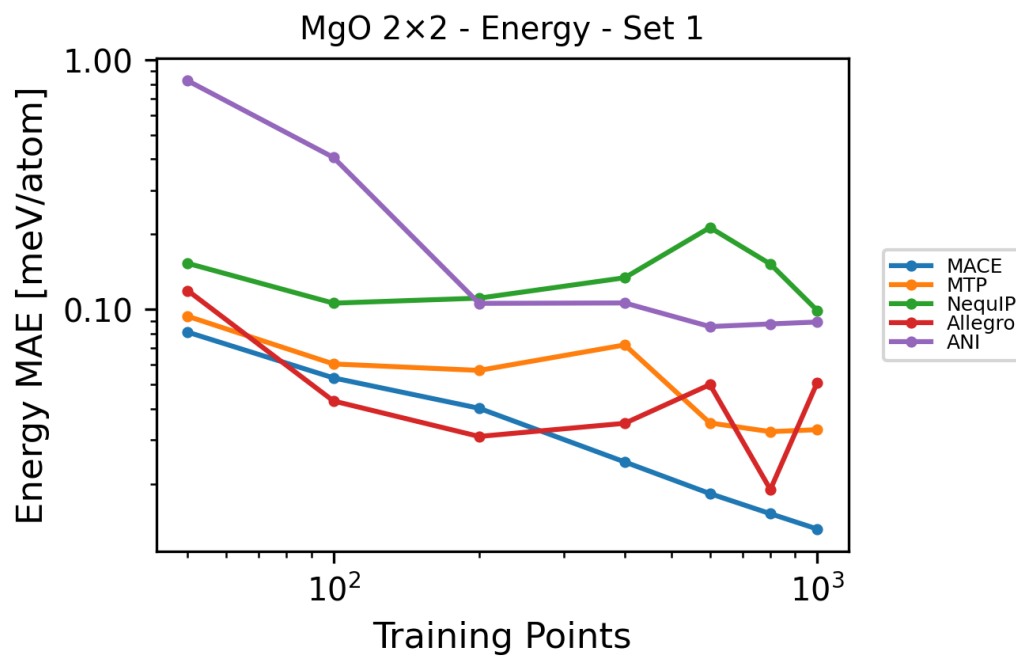
[#]*Department of Chemistry, The Chinese University of Hong Kong, New Territories, Shatin, Hong Kong 999077, P. R. China*

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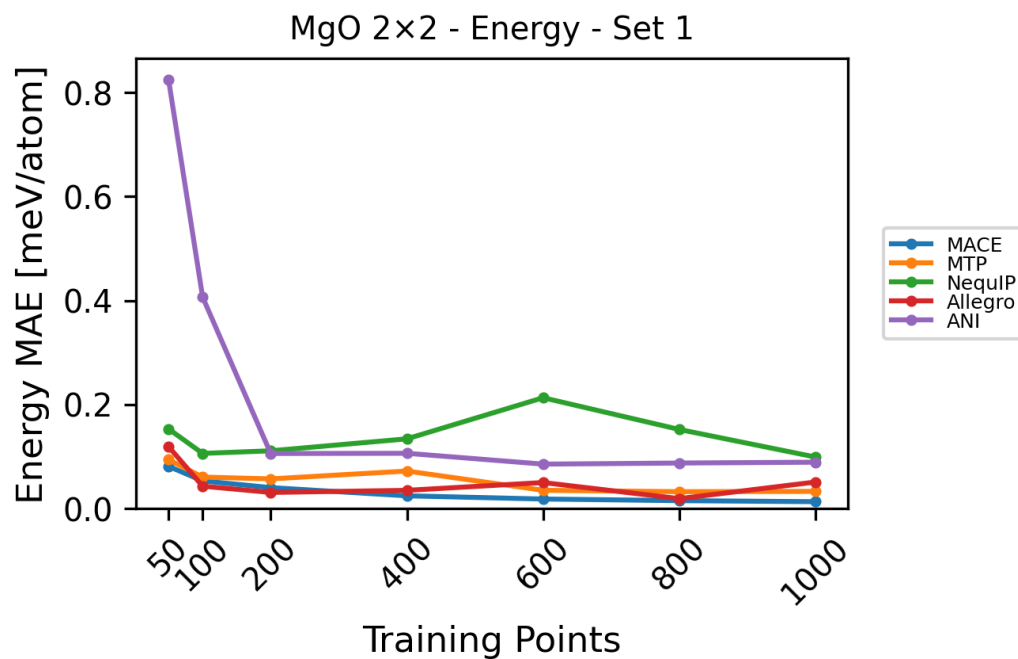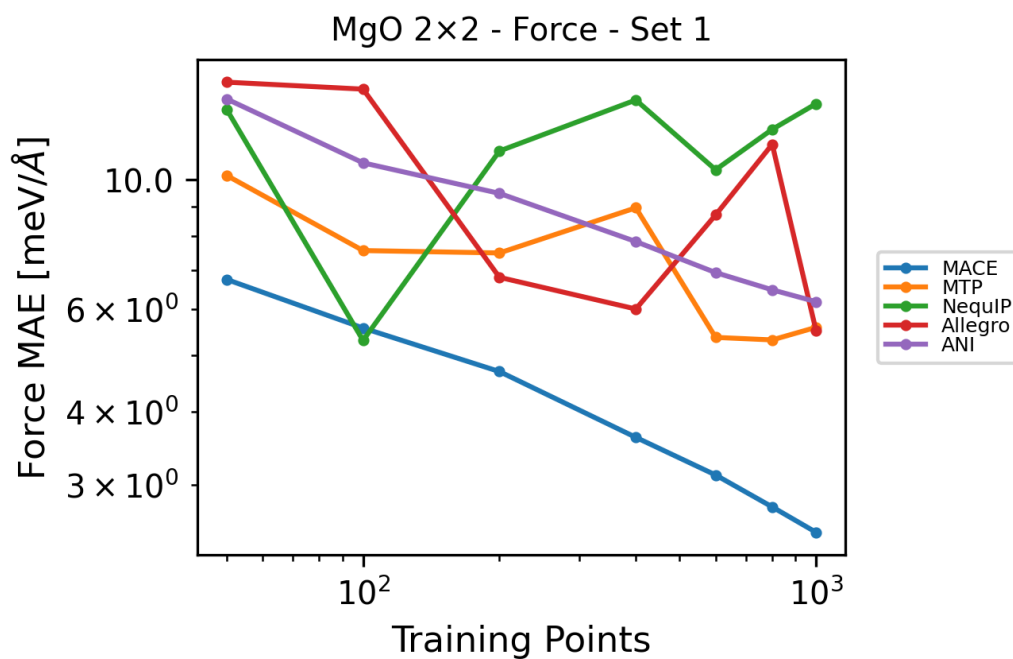
Data Learning Curves

MgO 2×2

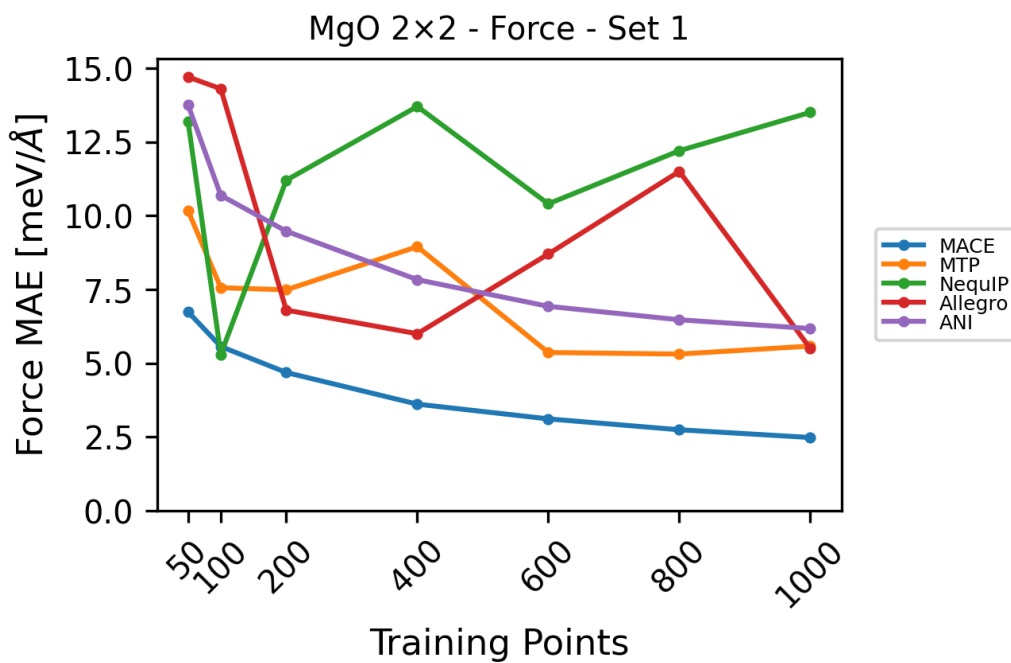**Figure S1.** Energy mean absolute error vs training points for MgO 2×2, Set 1. Unit: meV/atom.

Figure S2. Energy mean absolute error vs training points for MgO 2×2, Set 1. Unit: meV/atom.
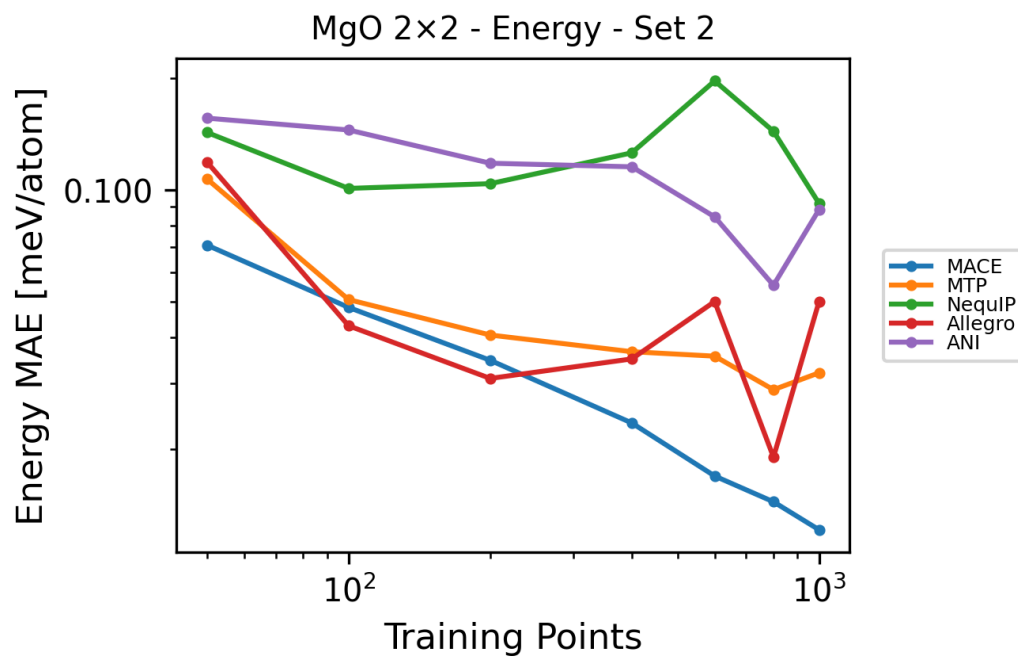
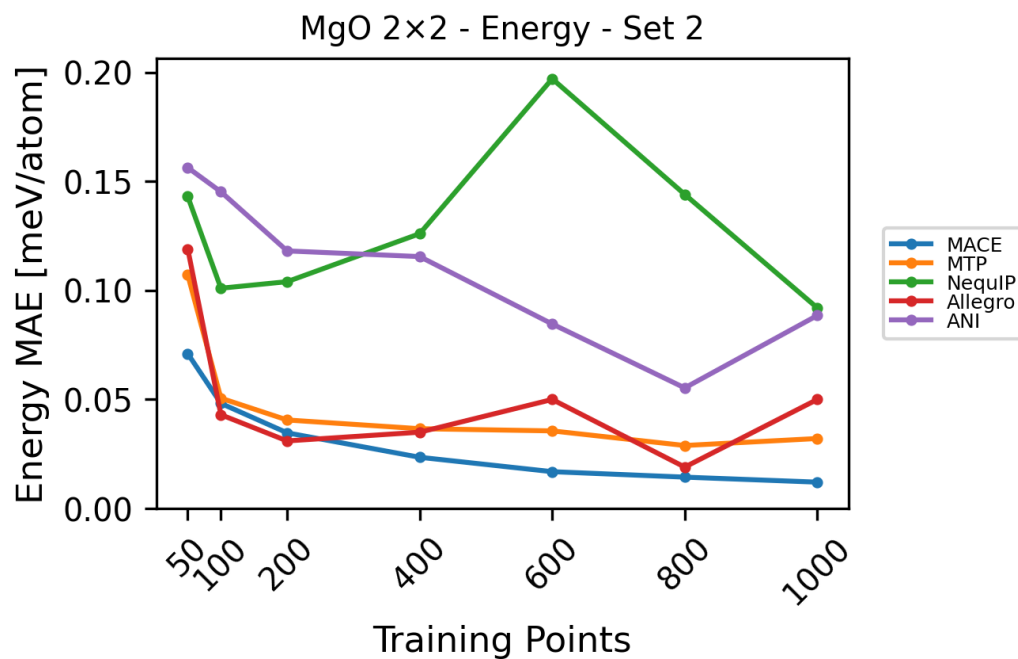**Figure S3.** Force mean absolute error vs training points for MgO 2×2, Set 1. Unit: meV/Å.
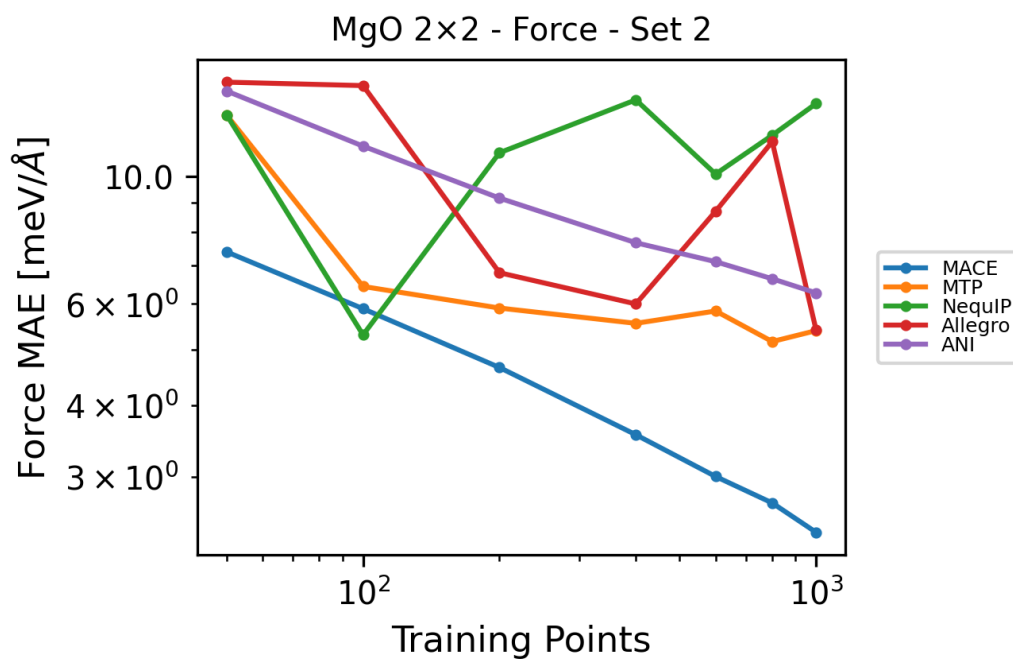
Figure S4. Force mean absolute error vs training points for MgO 2×2, Set 1. Unit: meV/Å.
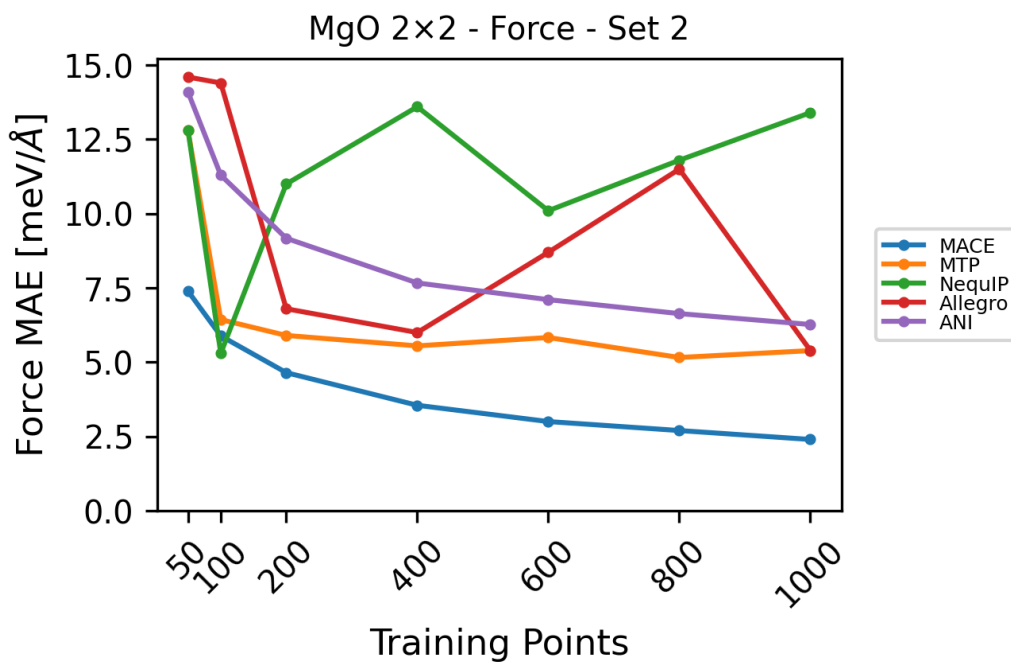
Figure S5. Energy mean absolute error vs training points for MgO 2×2, Set 2. Unit: meV/atom.
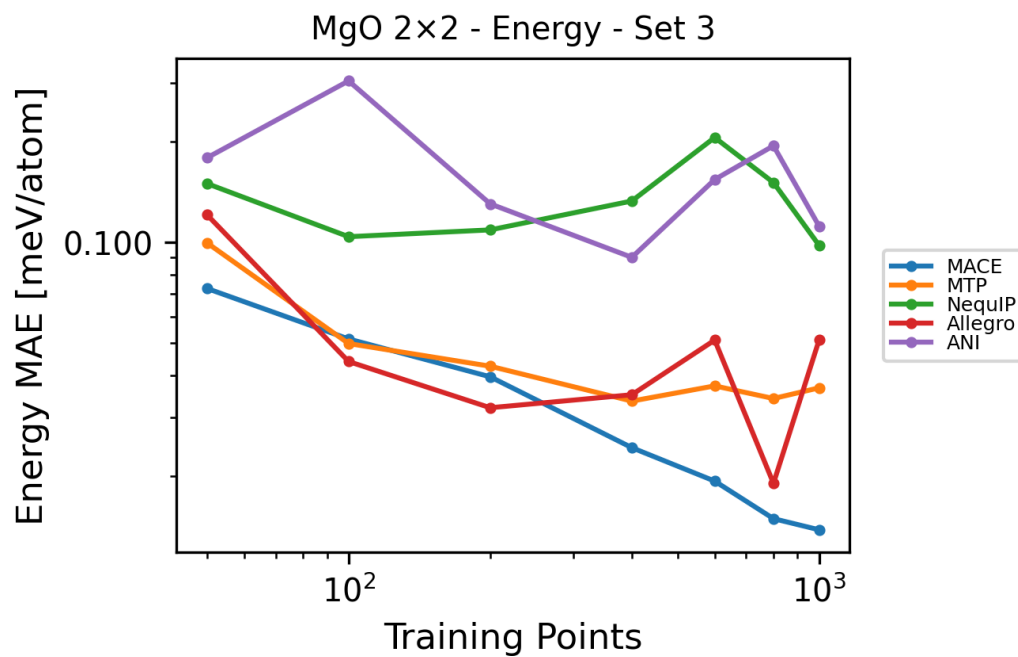
Figure S6. Energy mean absolute error vs training points for MgO 2×2, Set 2. Unit: meV/atom.
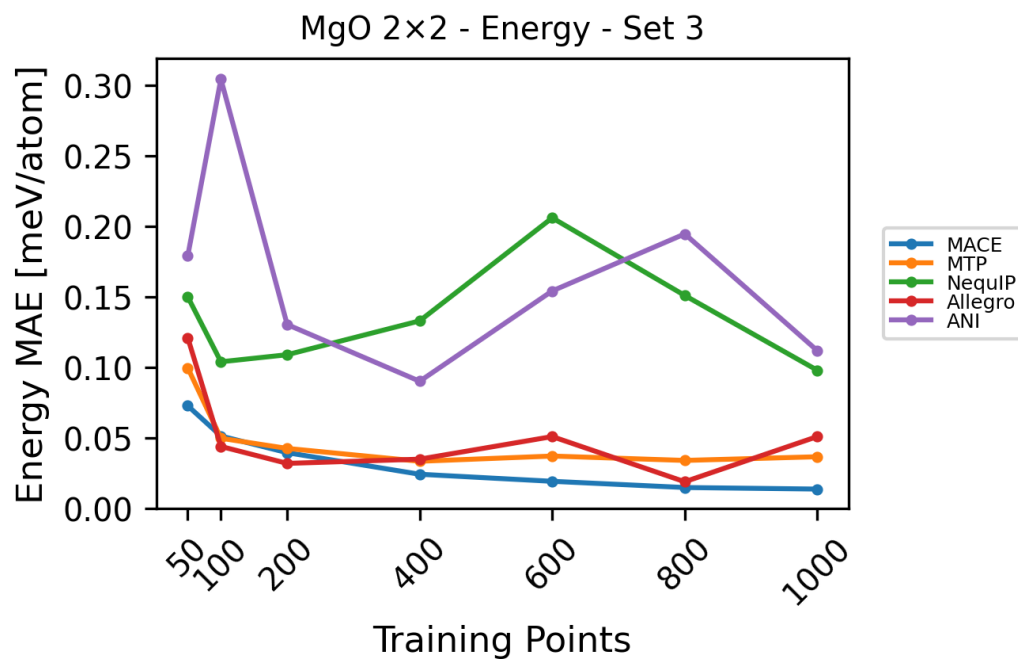
Figure S7. Force mean absolute error vs training points for MgO 2×2, Set 2. Unit: meV/Å.
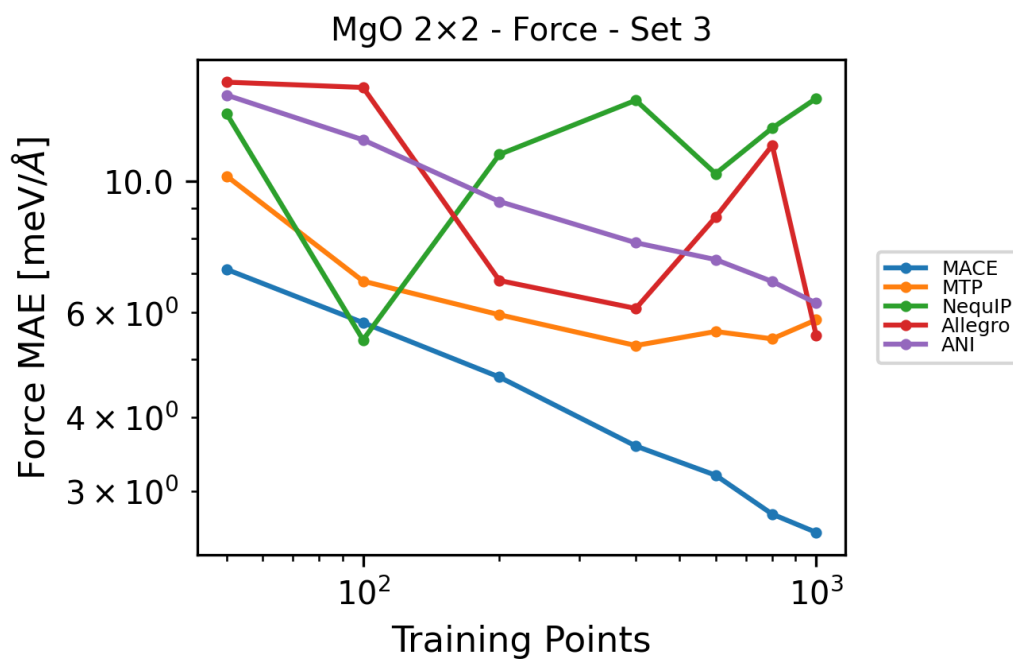
Figure S8. Force mean absolute error vs training points for MgO 2×2, Set 2. Unit: meV/Å.

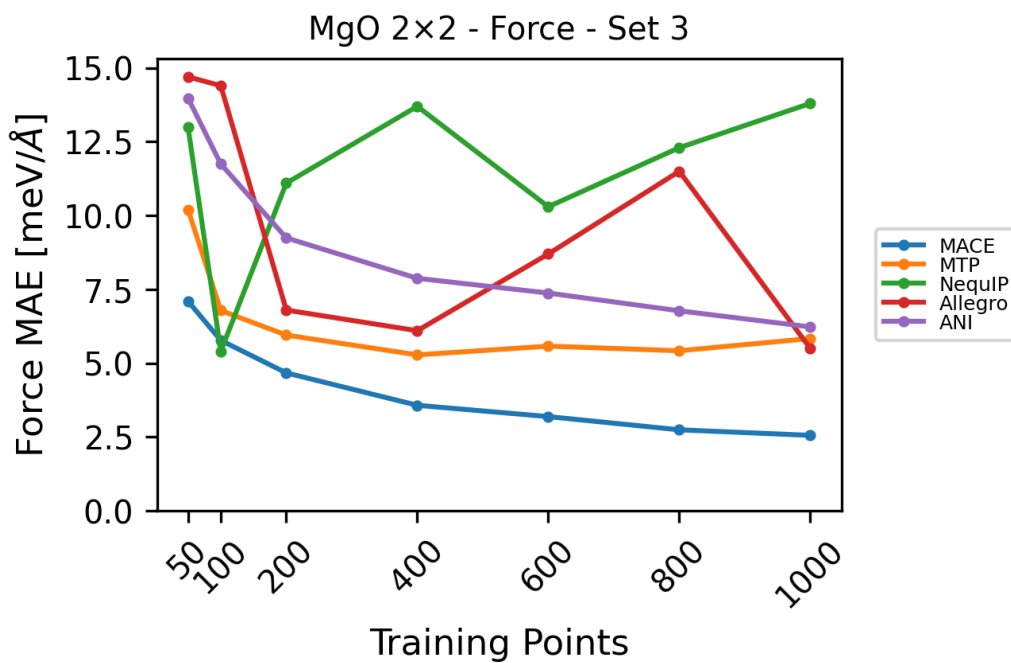**Figure S9.** Energy mean absolute error vs training points for MgO 2×2, Set 3. Unit: meV/atom.

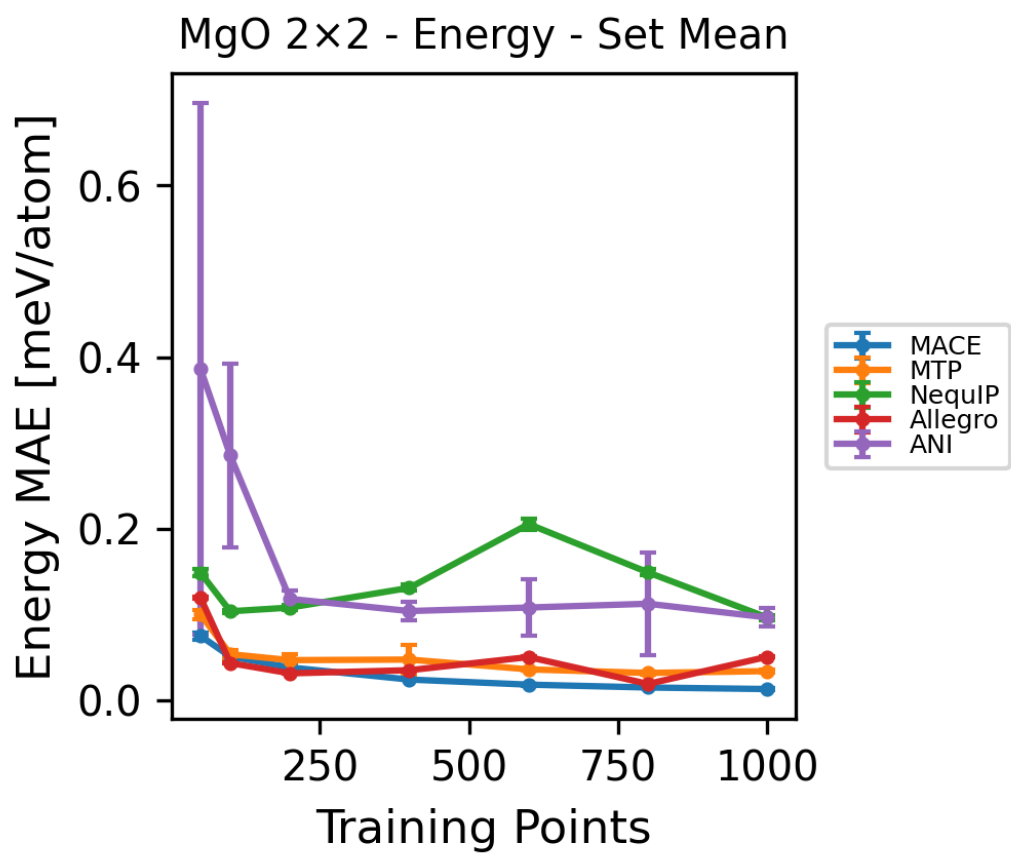**Figure S10.** Energy mean absolute error vs training points for MgO 2×2, Set 3. Unit: meV/atom.

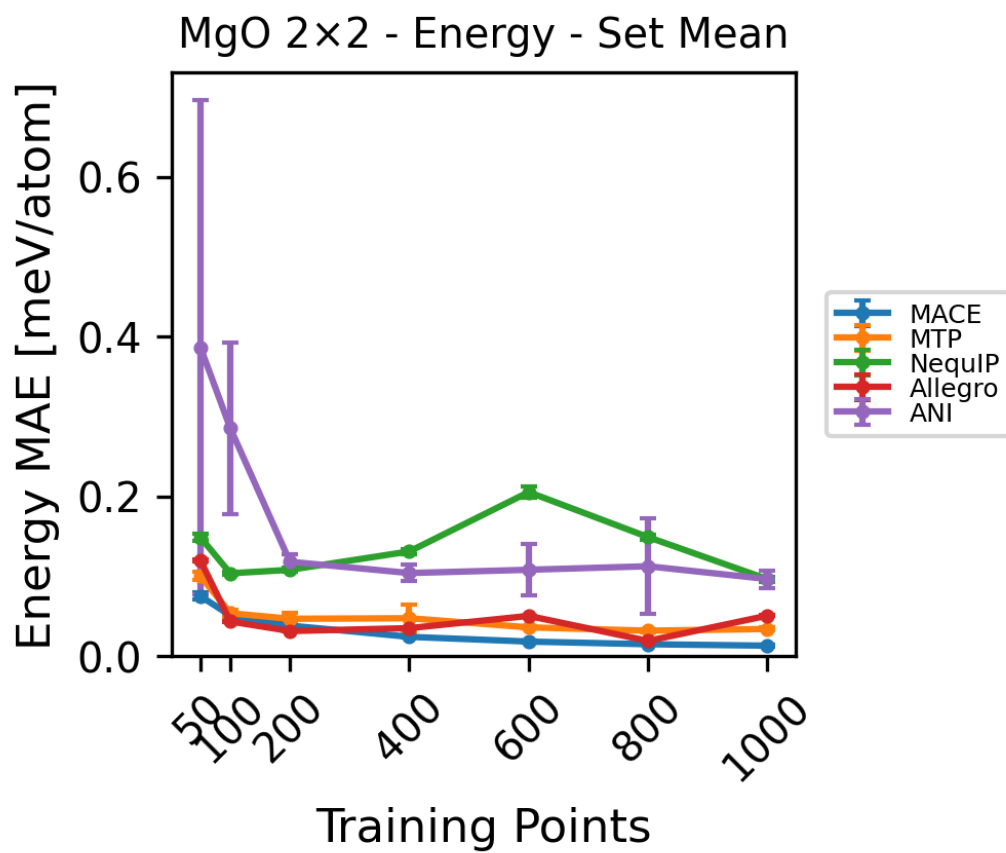**Figure S11.** Force mean absolute error vs training points for MgO 2×2, Set 3. Unit: meV/Å.
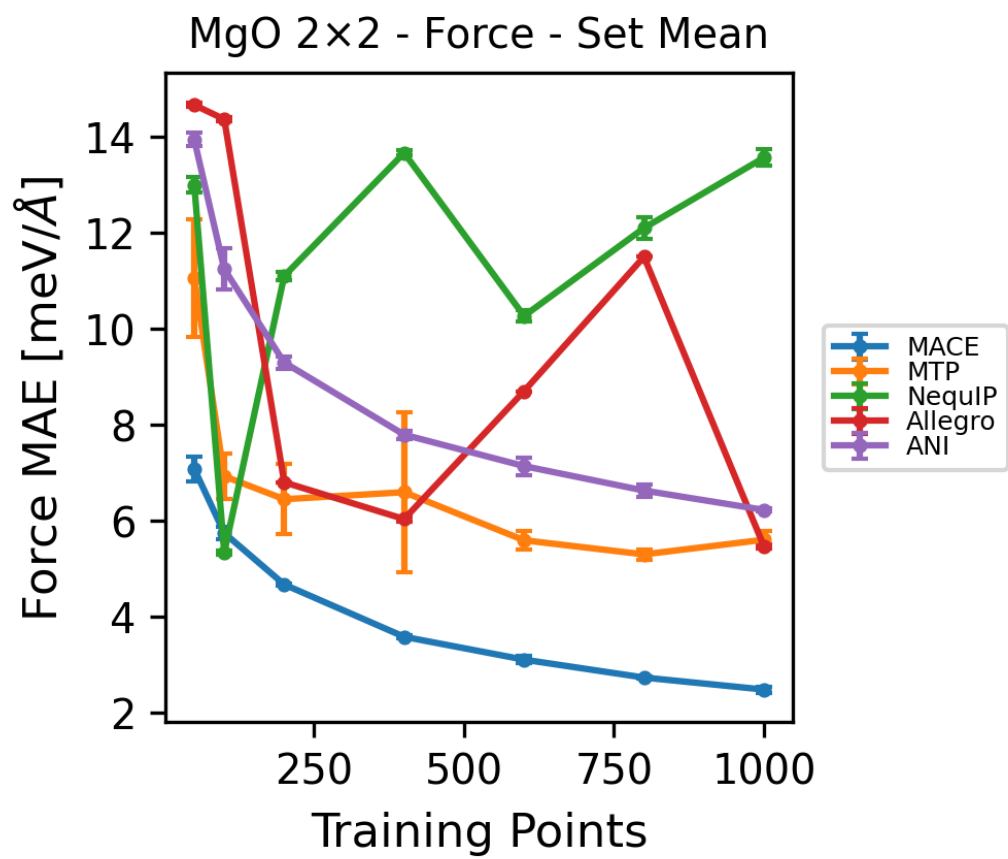
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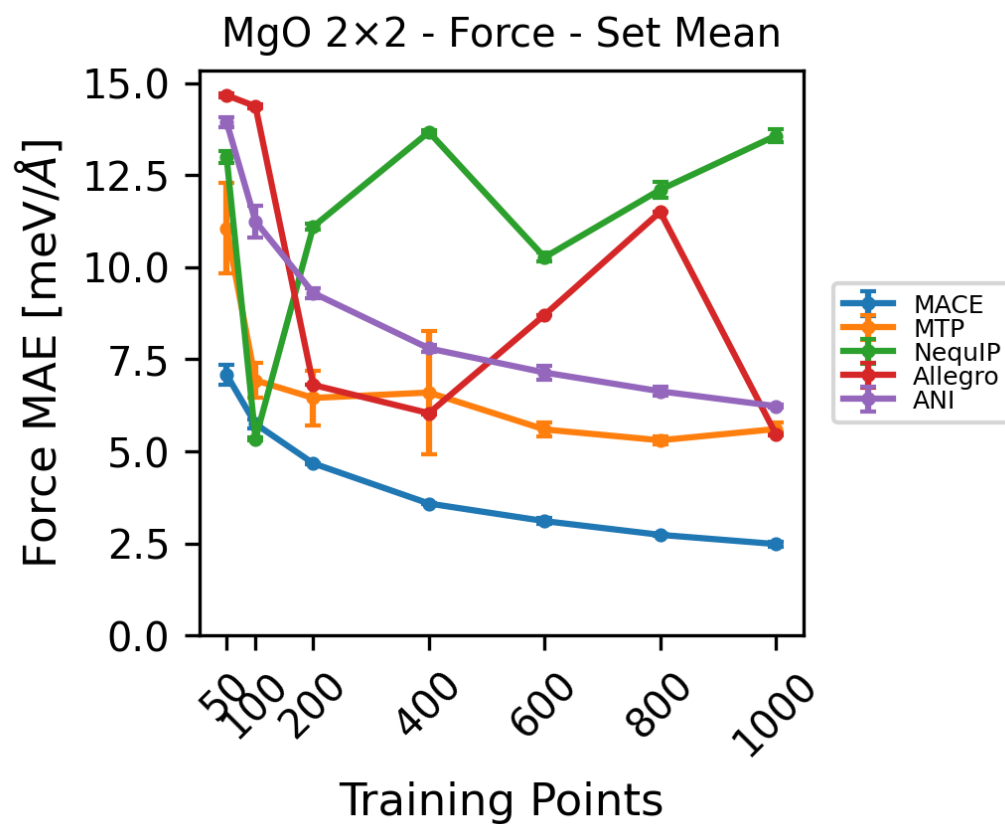
Figure S13. Energy mean absolute error vs training points for MgO 2×2, Set mean. Unit: meV/atom.

Figure S14. Energy mean absolute error vs training points for MgO 2×2, Set mean. Unit: meV/atom.
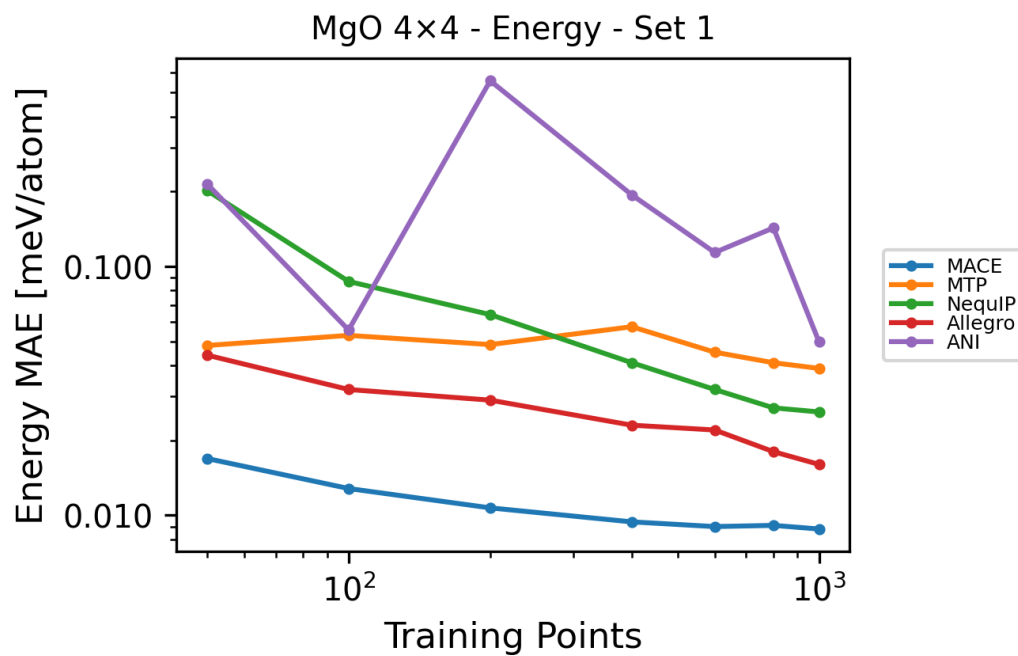
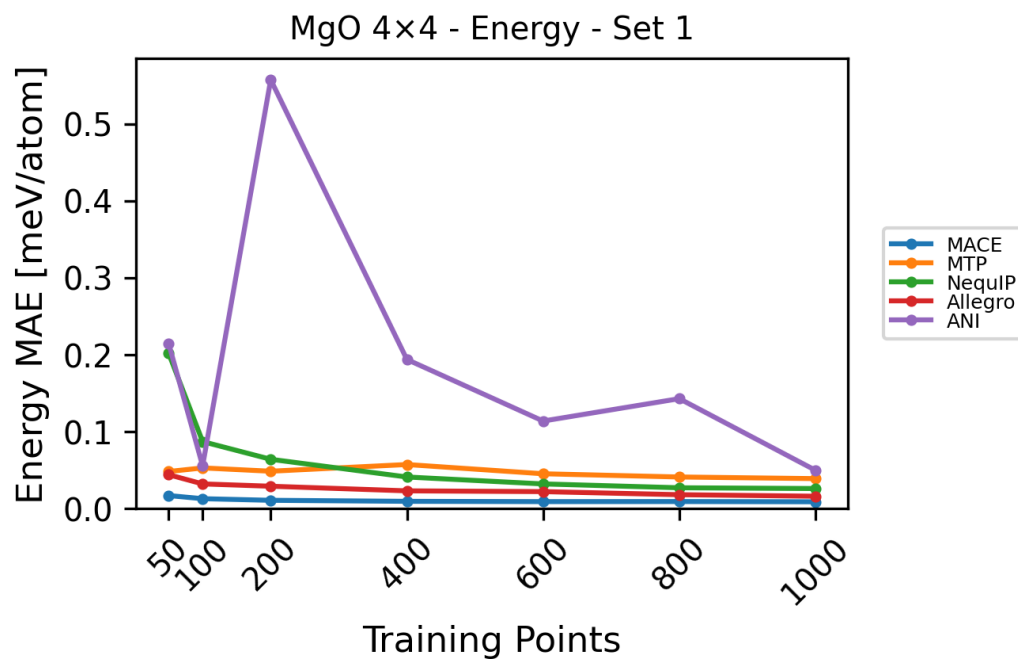**Figure S15.** Force mean absolute error vs training points for MgO 2×2, Set mean. Unit: meV/Å.

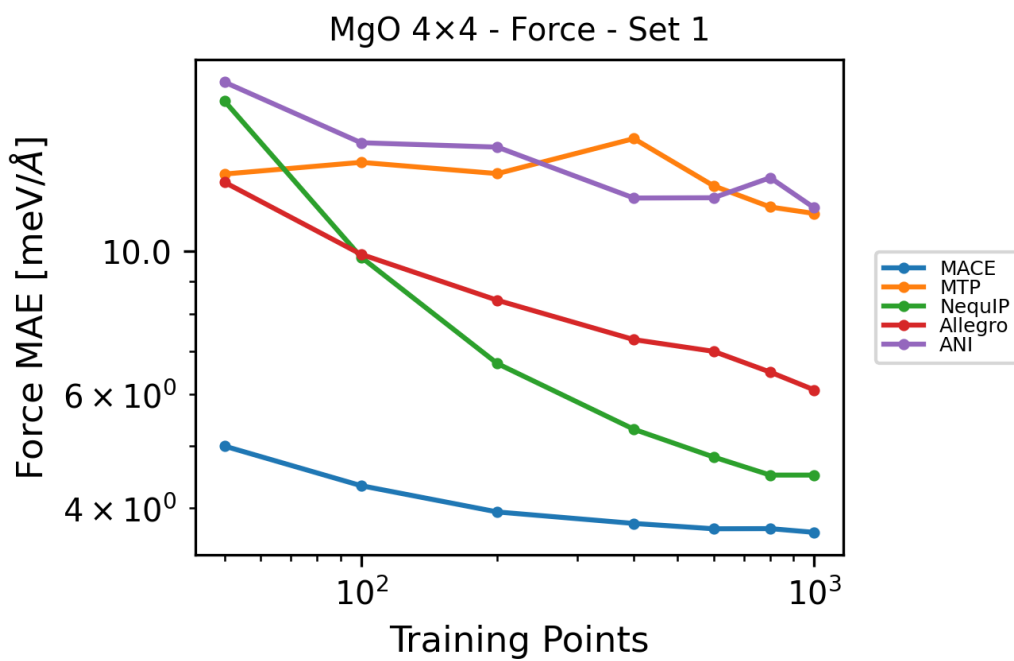**Figure S16.** Force mean absolute error vs training points for MgO 2×2, Set mean. Unit: meV/Å.

MgO 4×4

Figure S17. Energy mean absolute error vs training points for MgO 4×4, Set 1. Unit: meV/atom.
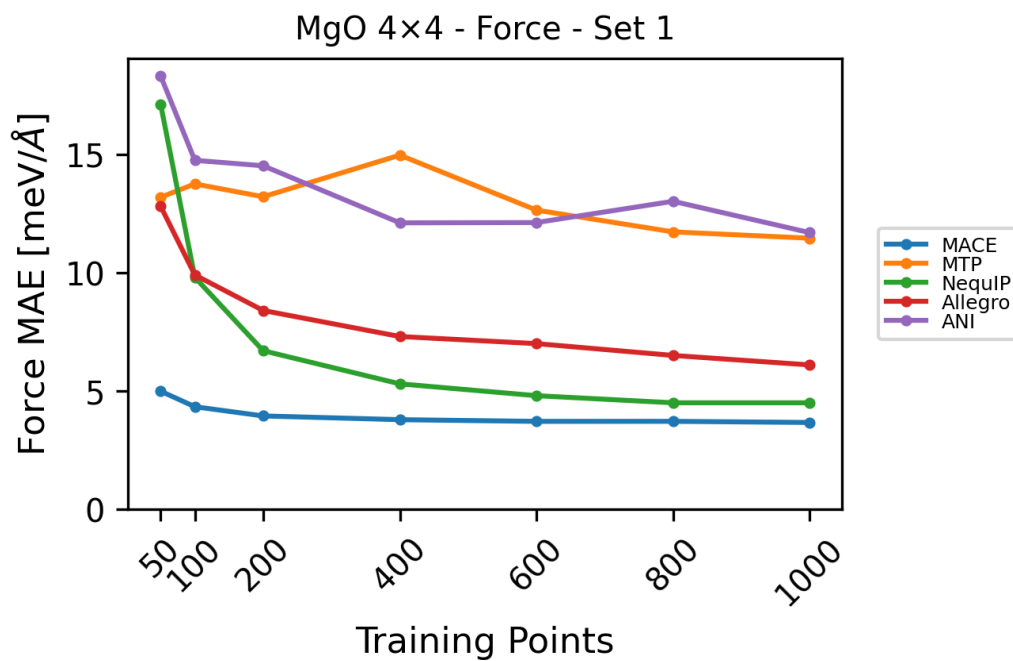
Figure S18. Energy mean absolute error vs training points for MgO 4×4, Set 1. Unit: meV/atom.
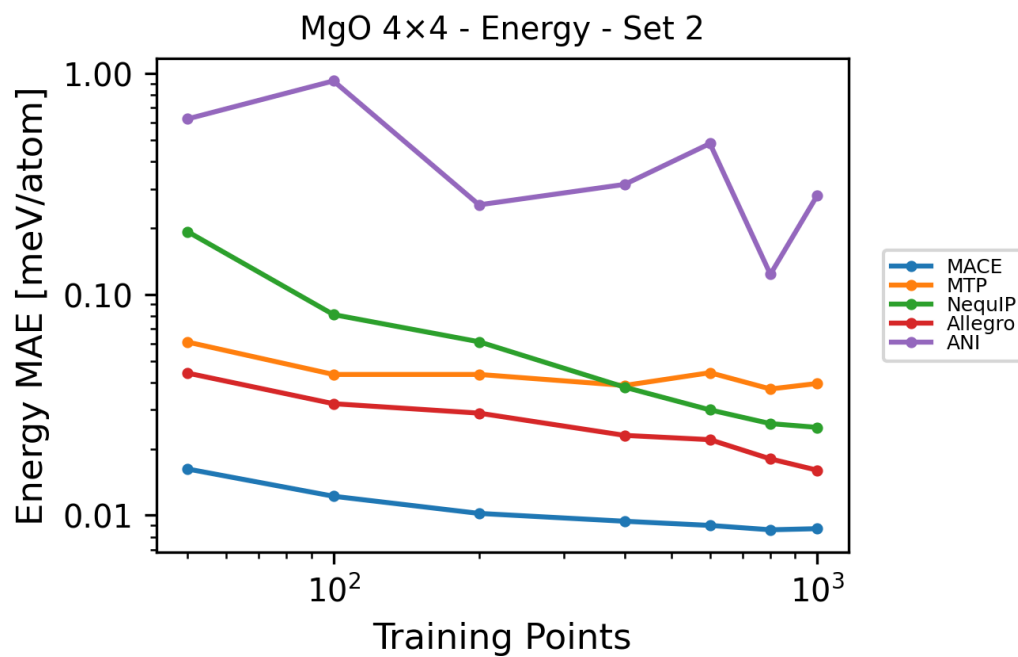
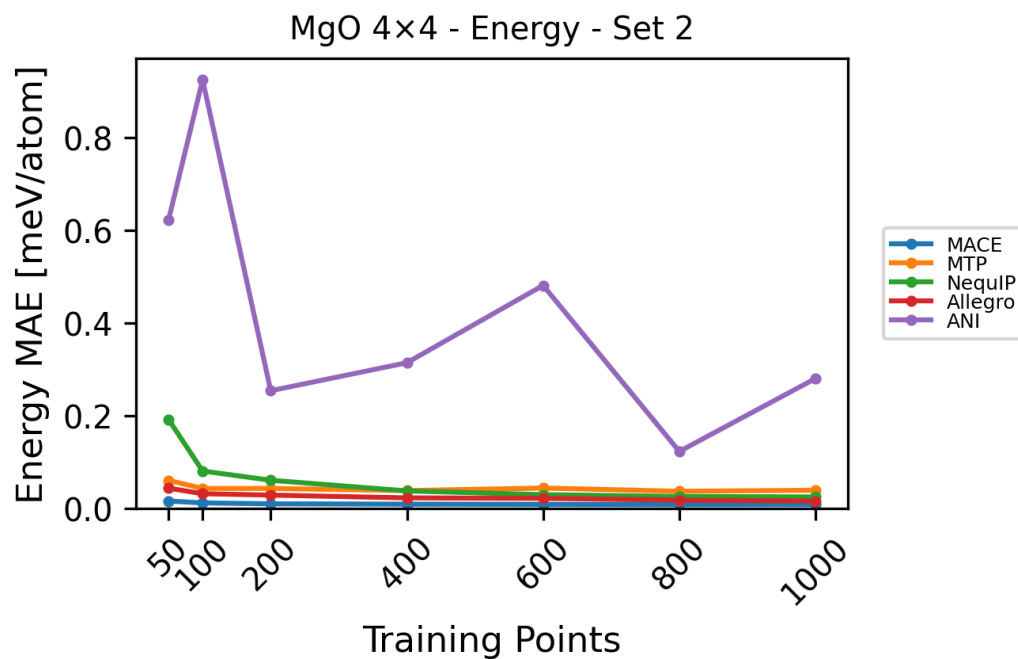**Figure S19.** Force mean absolute error vs training points for MgO 4×4, Set 1. Unit: meV/Å.
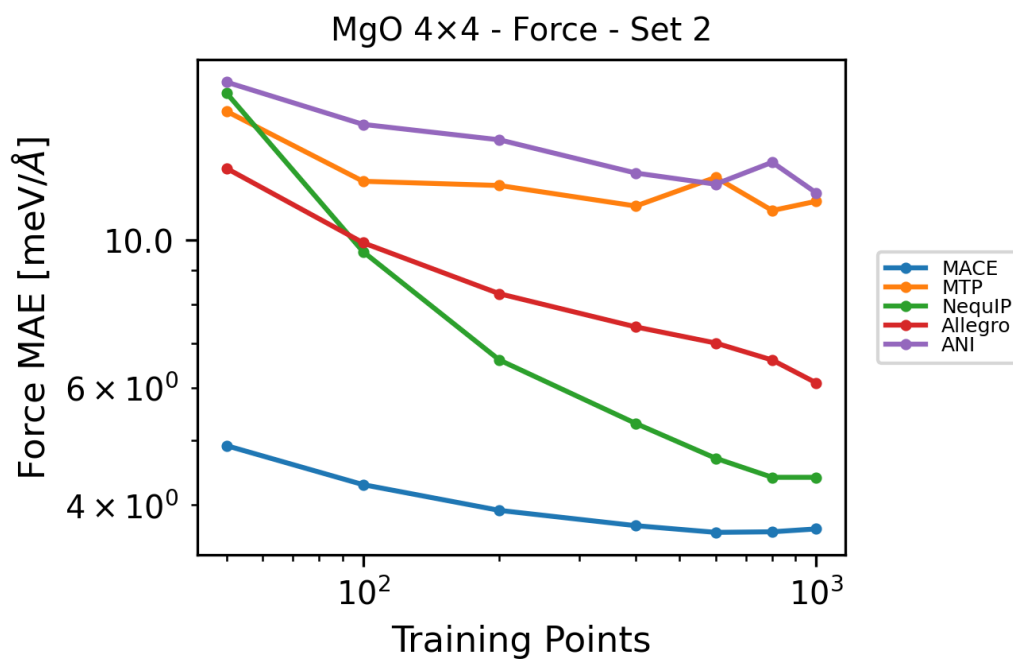
Figure S20. Force mean absolute error vs training points for MgO 4×4, Set 1. Unit: meV/Å.
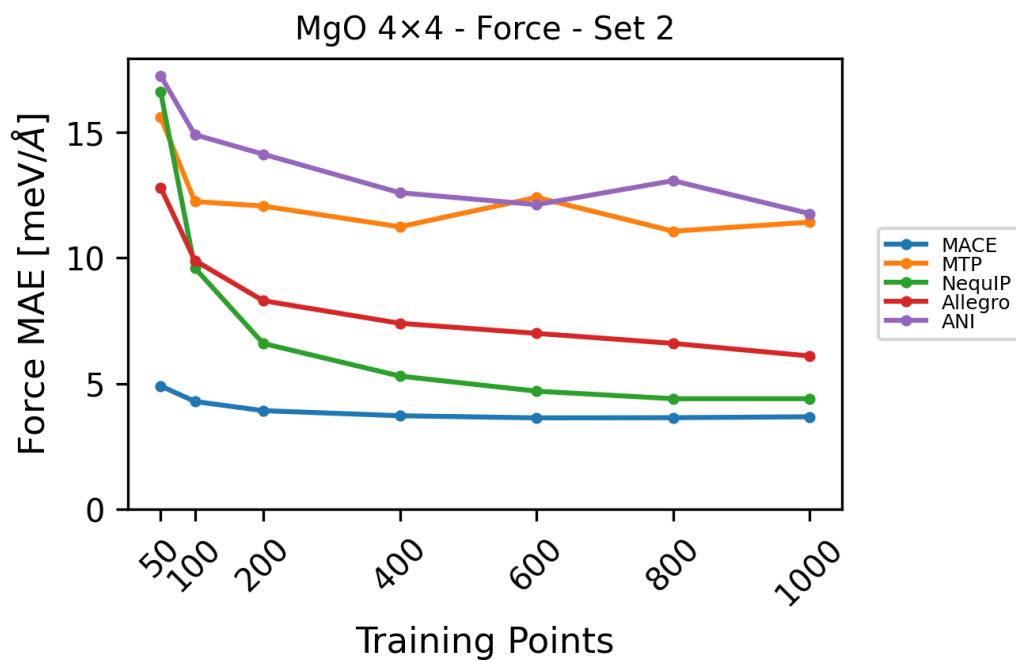
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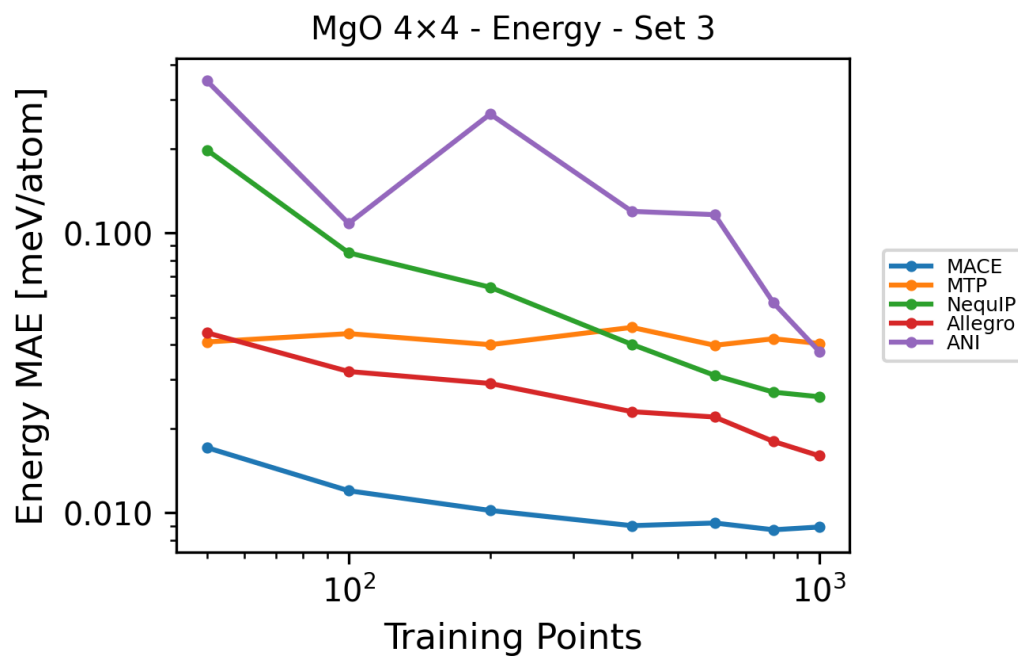
Figure S22. Energy mean absolute error vs training points for MgO 4×4, Set 2. Unit: meV/atom.
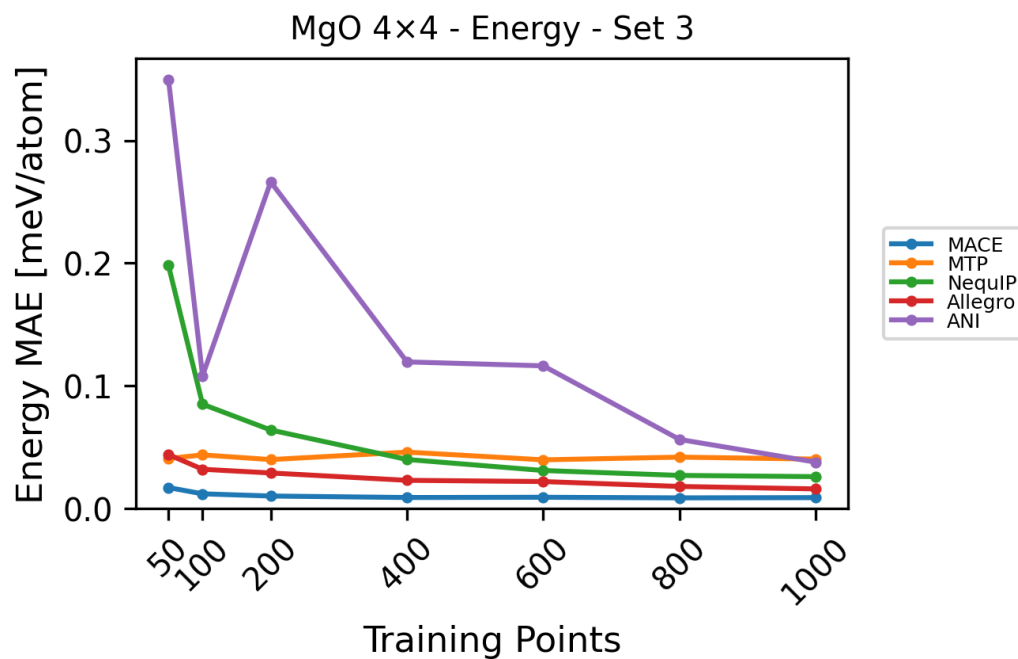
Figure S23. Force mean absolute error vs training points for MgO 4×4, Set 2. Unit: meV/Å.
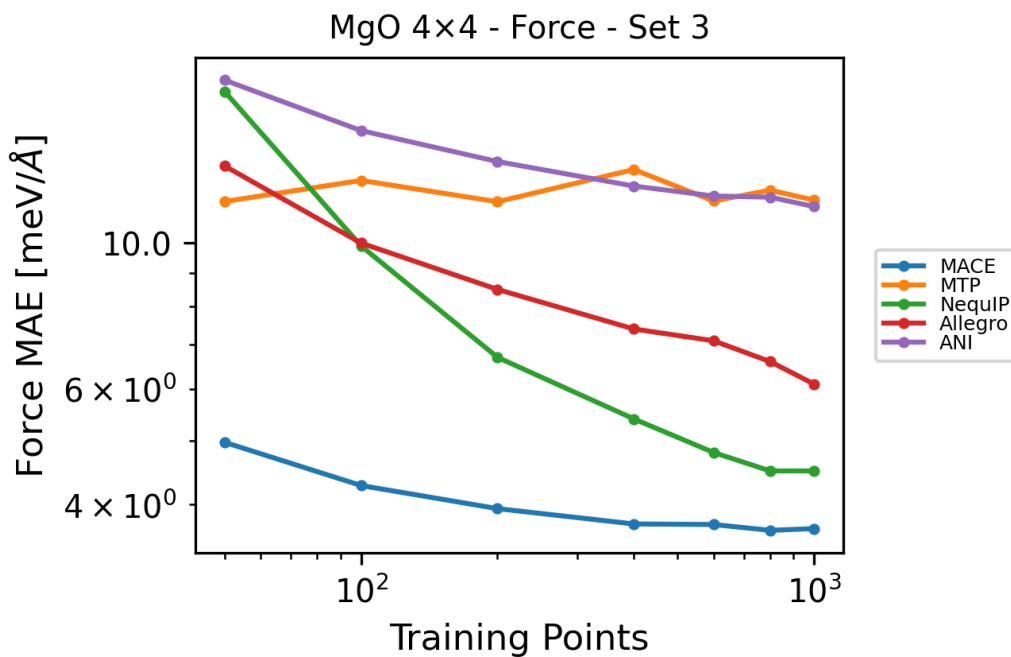
Figure S24. Force mean absolute error vs training points for MgO 4×4, Set 2. Unit: meV/Å.

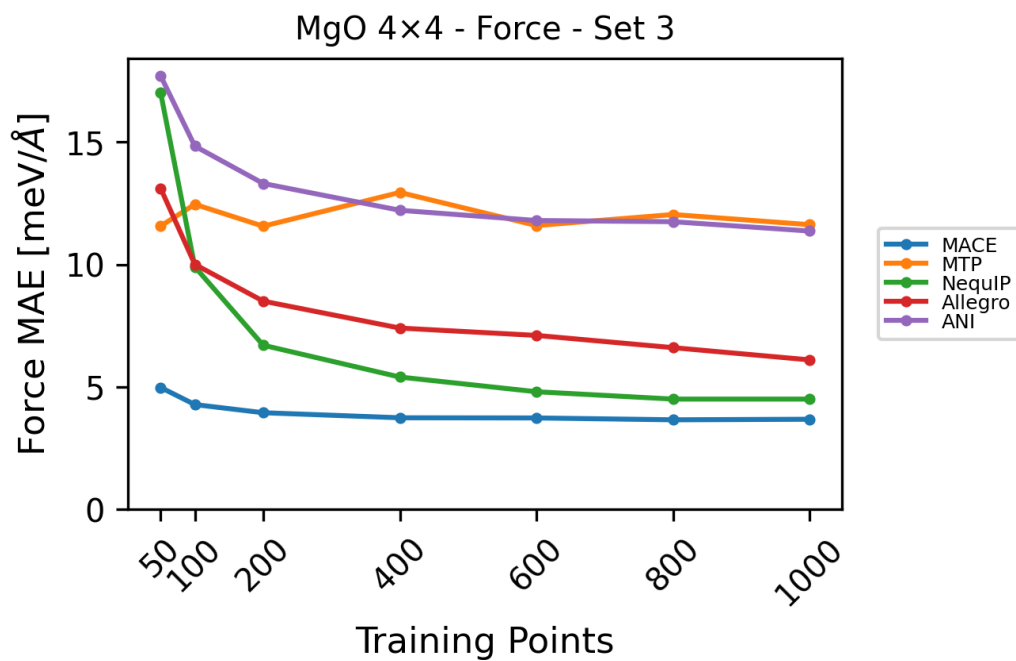**Figure S25.** Energy mean absolute error vs training points for MgO 4×4, Set 3. Unit: meV/atom.

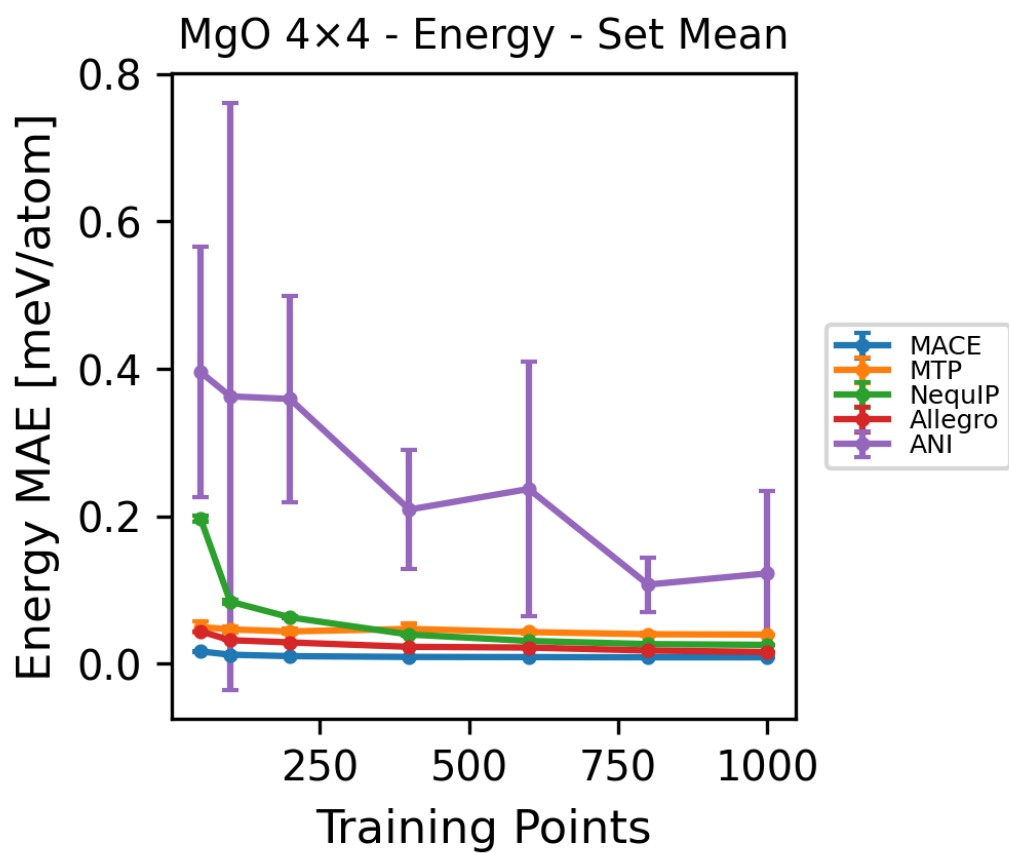**Figure S26.** Energy mean absolute error vs training points for MgO 4×4, Set 3. Unit: meV/atom.

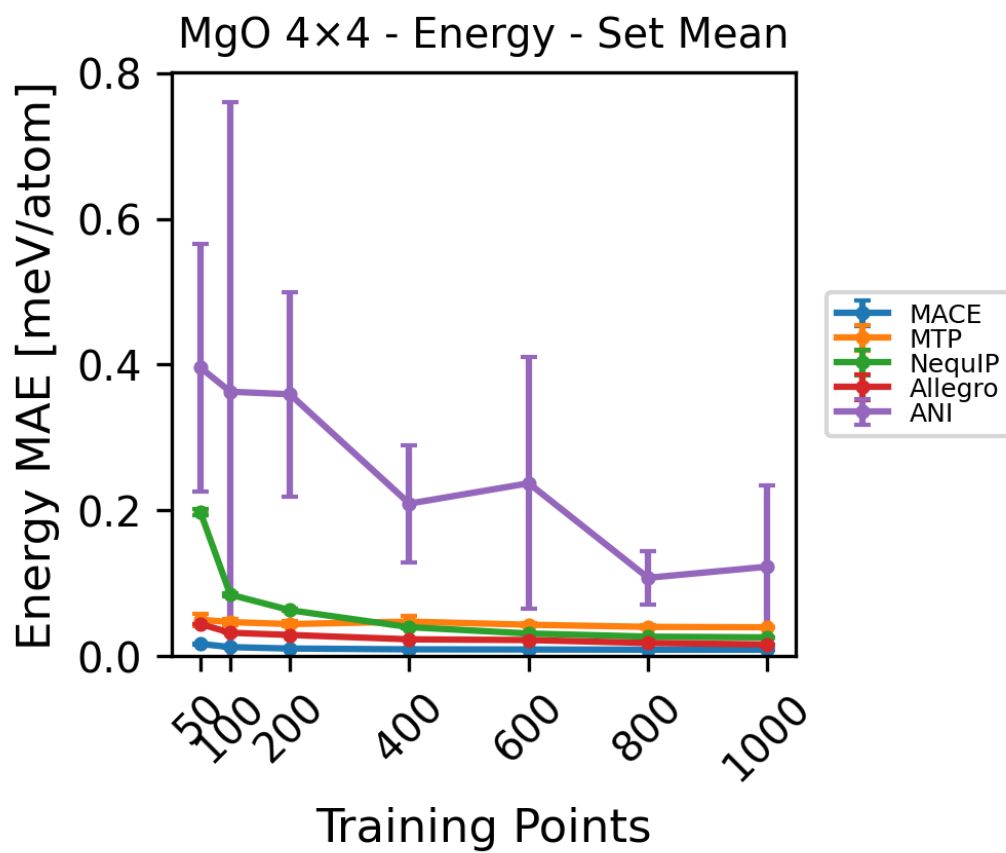**Figure S27.** Force mean absolute error vs training points for MgO 4×4, Set 3. Unit: meV/Å.
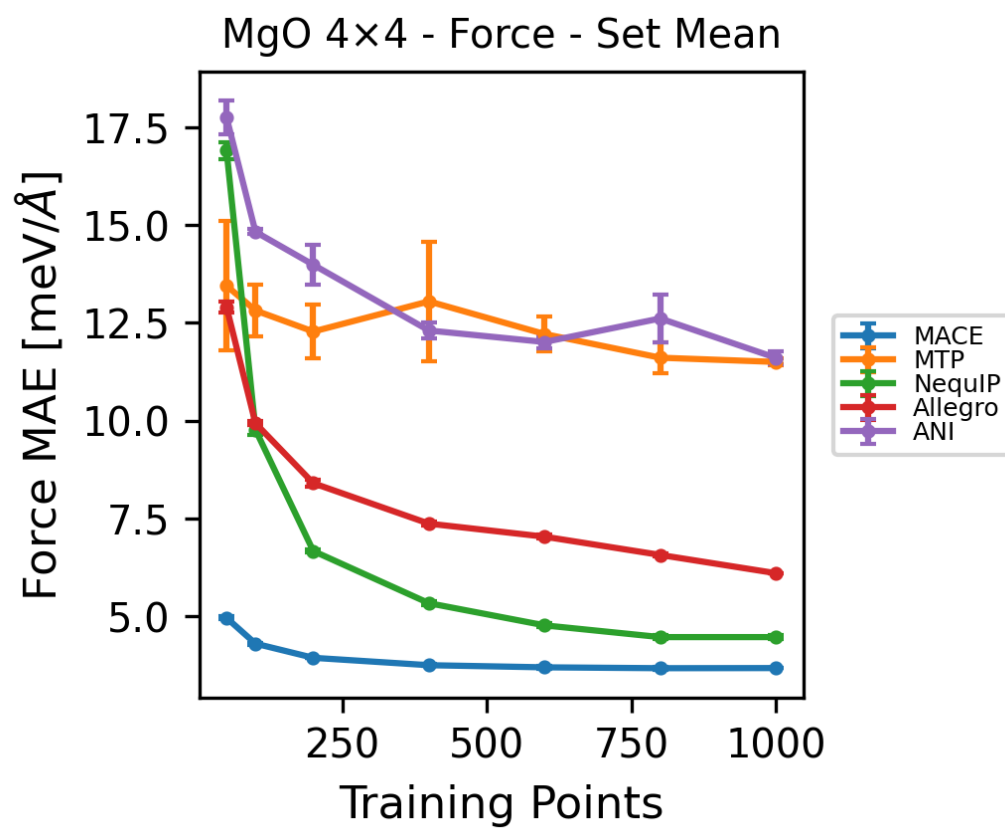
Figure S28. Force mean absolute error vs training points for MgO 4×4, Set 3. Unit: meV/Å.
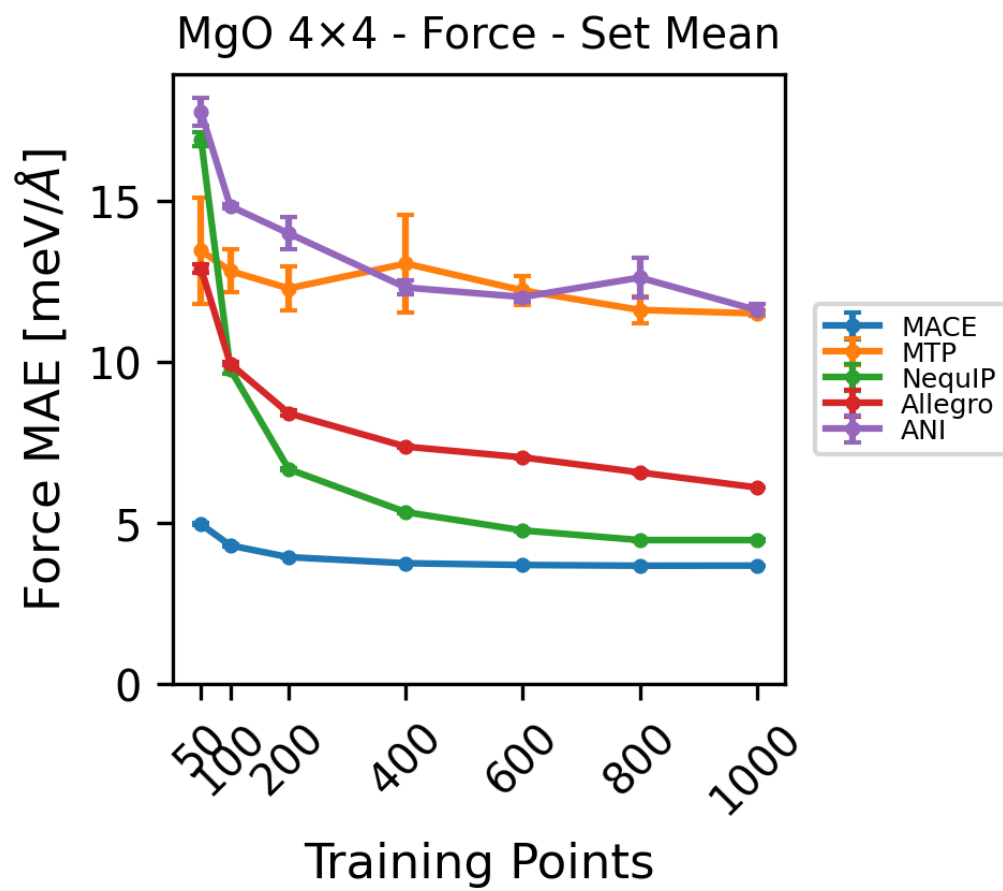
Figure S29. Energy mean absolute error vs training points for MgO 4×4, Set mean. Unit: meV/atom.

Figure S30. Energy mean absolute error vs training points for MgO 4×4, Set mean. Unit: meV/atom.
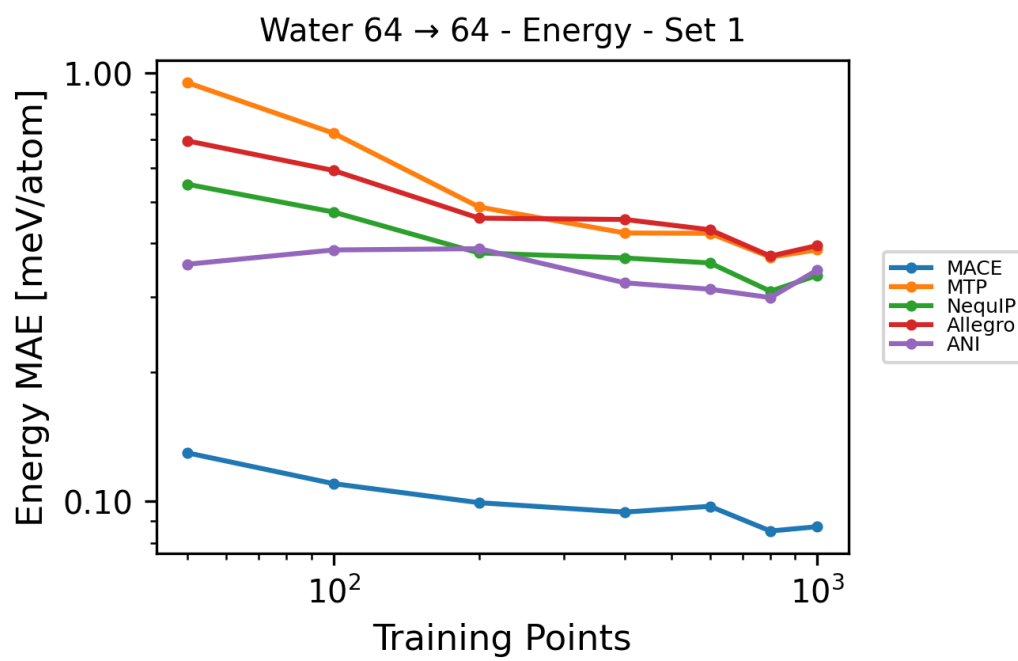
Figure S31. Force mean absolute error vs training points for MgO 4×4, Set mean. Unit: meV/Å.
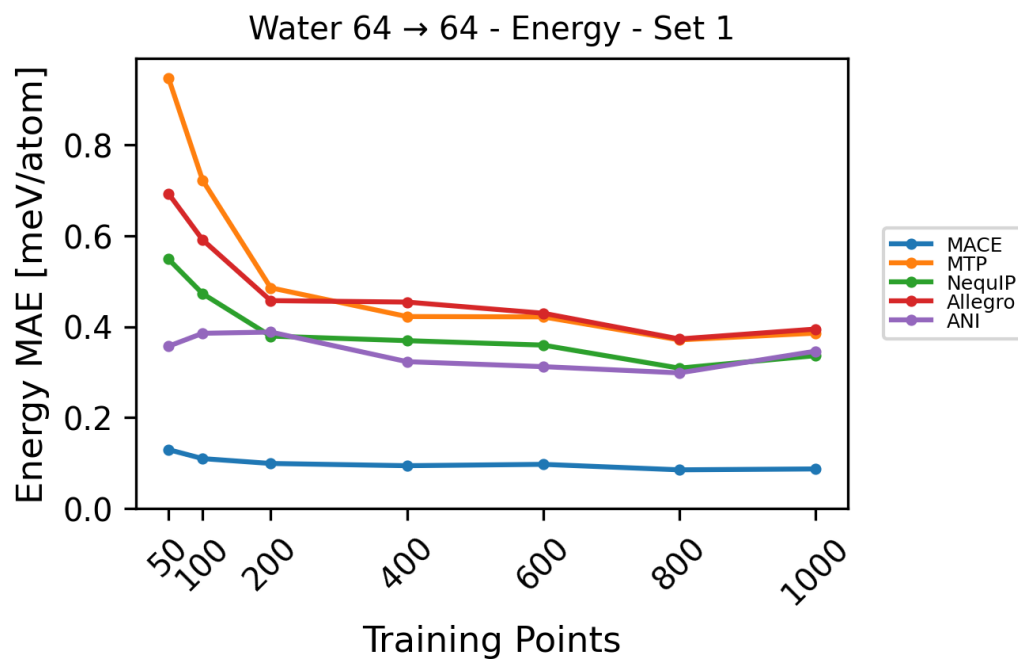
Figure S32. Force mean absolute error vs training points for MgO 4×4, Set mean. Unit: meV/Å.
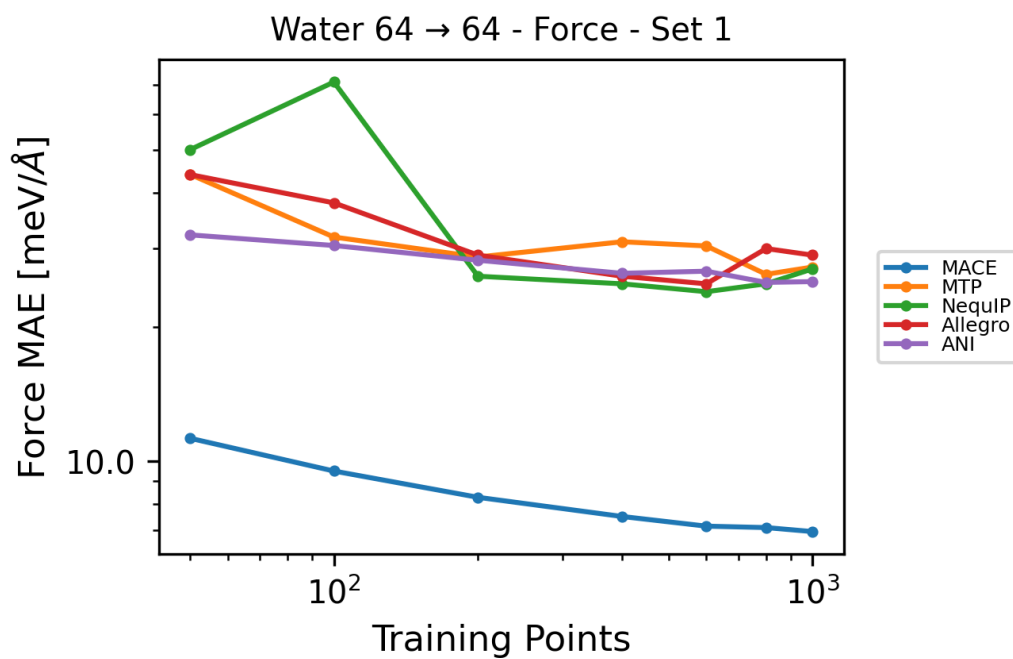
Water 64

Figure S33. Energy mean absolute error vs training points for Water 64, Set 1. Unit: meV/atom.
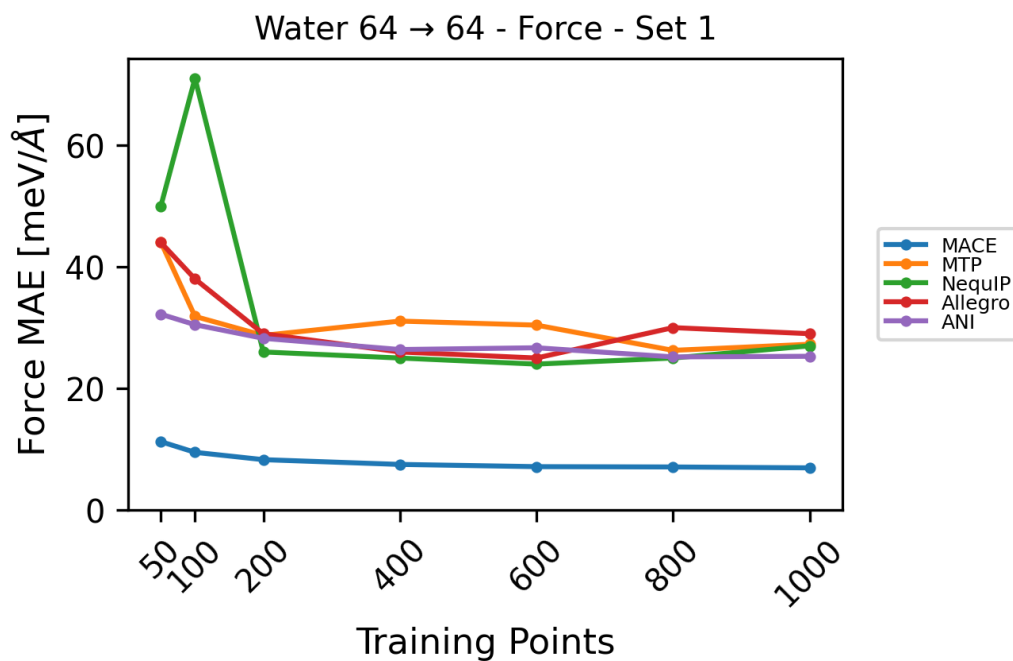
Figure S34. Energy mean absolute error vs training points for Water 64, Set 1. Unit: meV/atom.
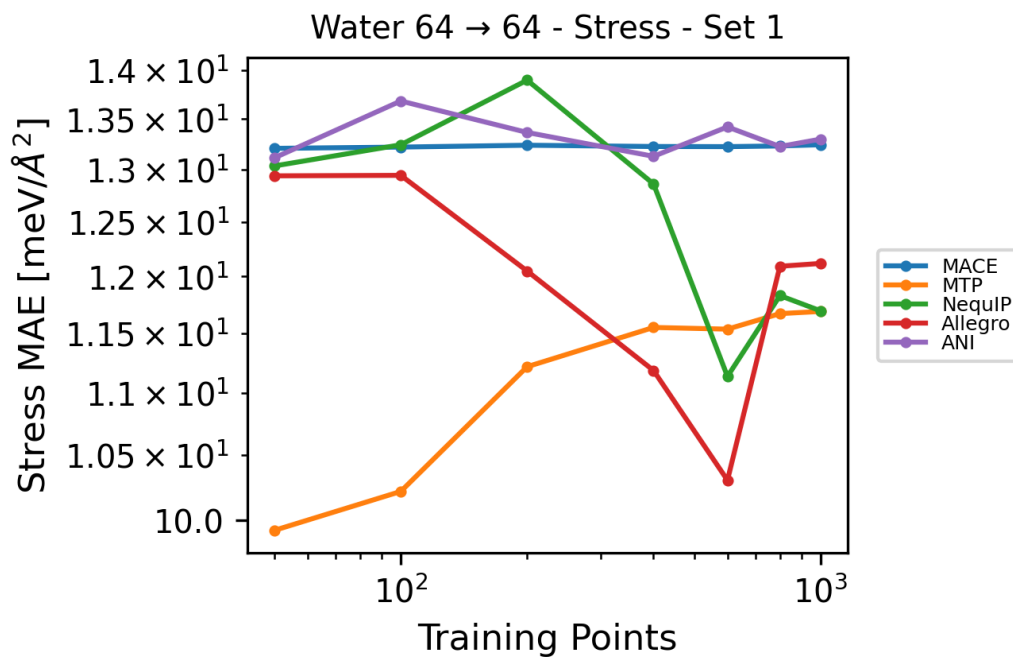
Figure S35. Force mean absolute error vs training points for Water 64, Set 1. Unit: meV/Å.
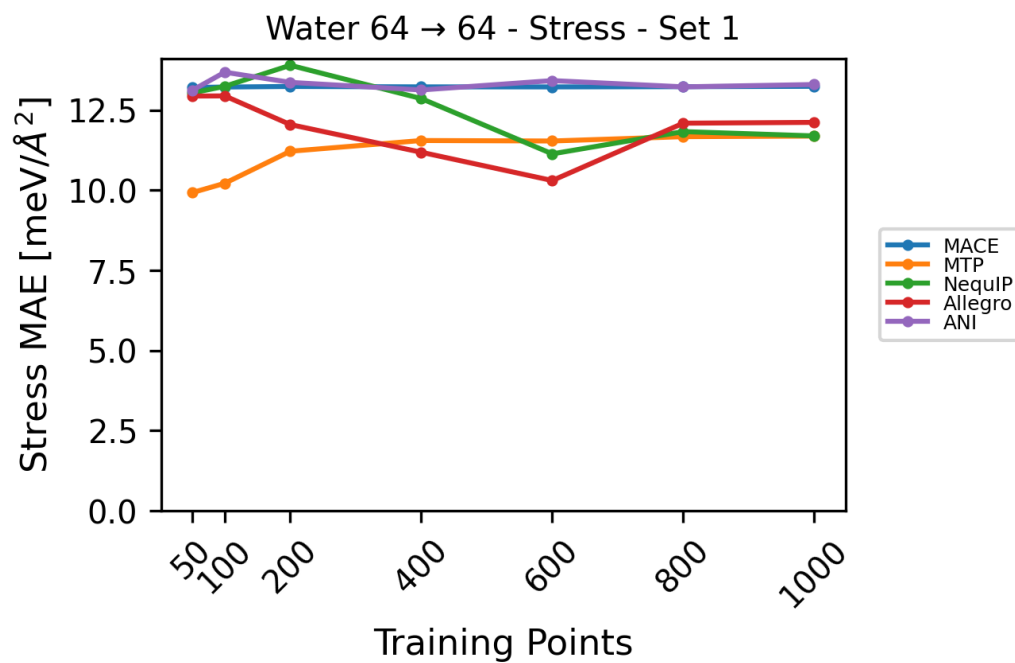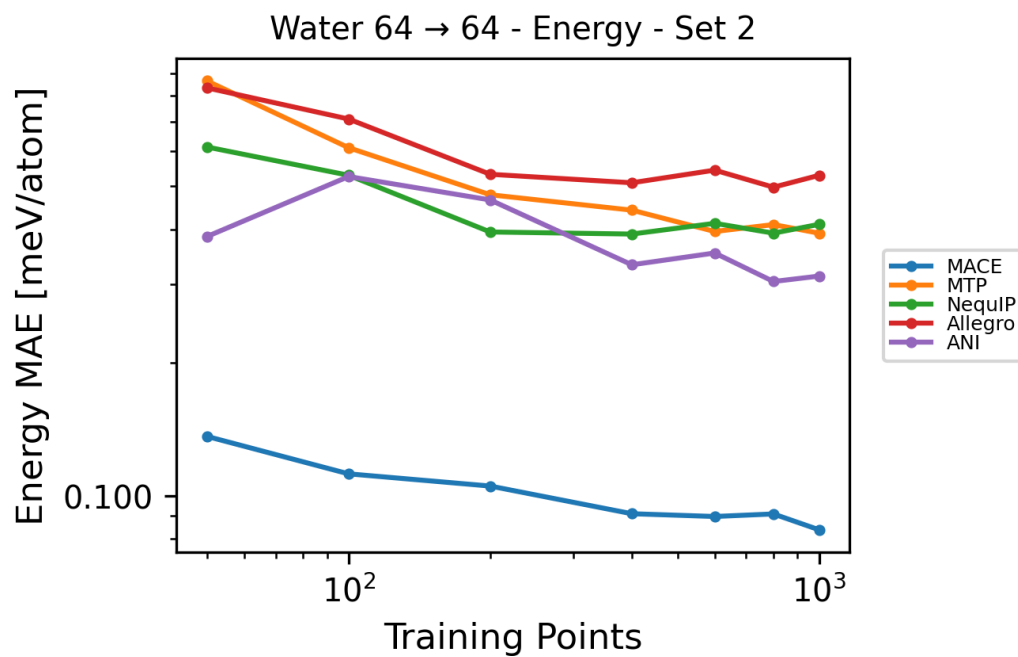
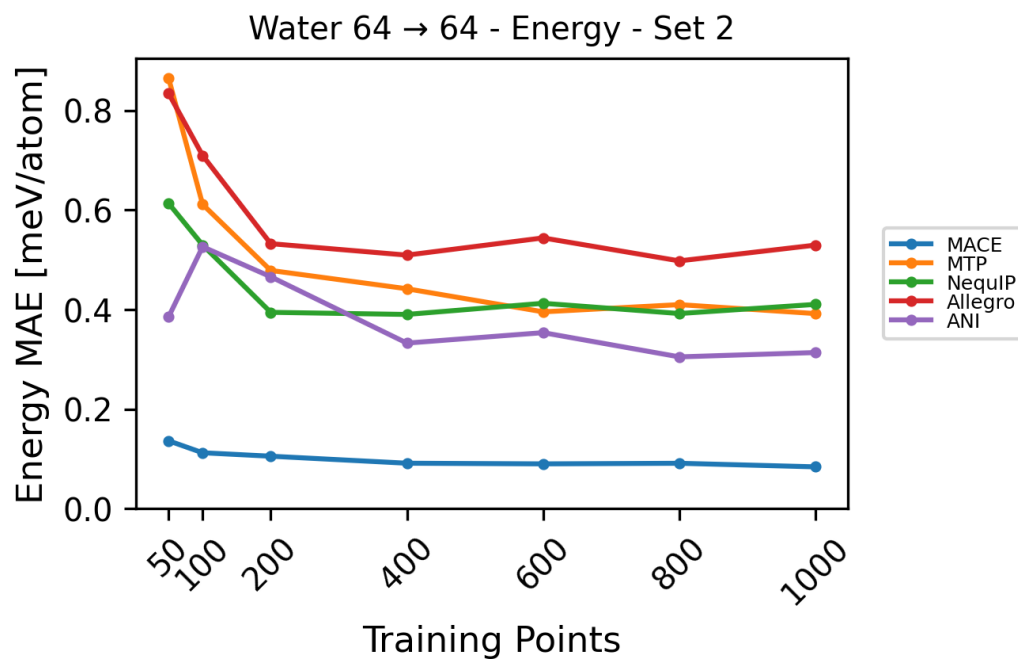**Figure S36.** Force mean absolute error vs training points for Water 64, Set 1. Unit: meV/Å.

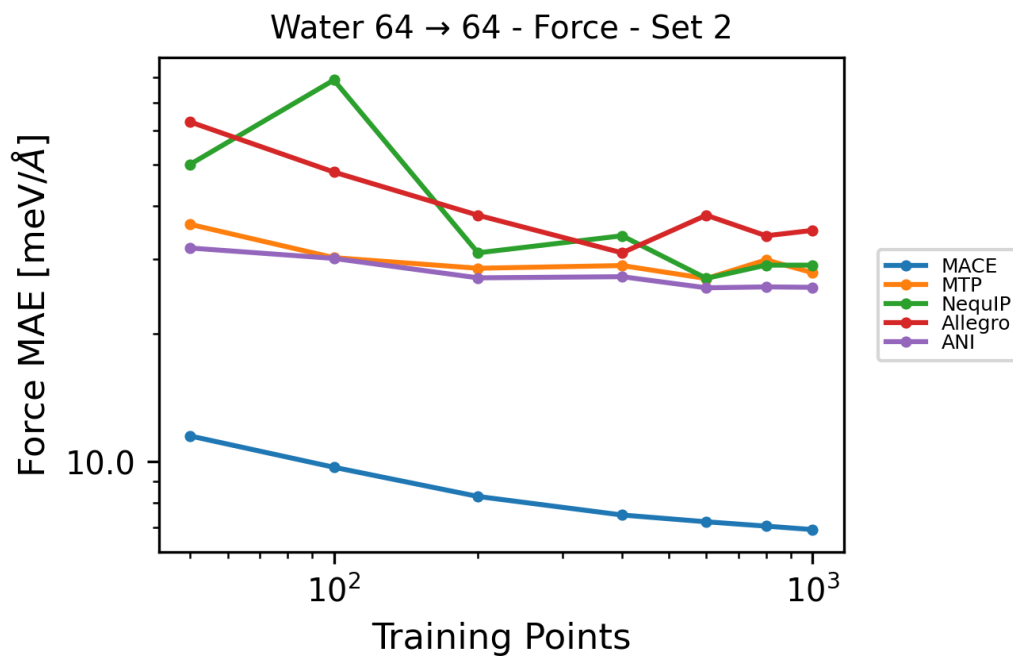**Figure S37.** Stress mean absolute error vs training points for Water 64, Set 1. Unit: meV/Å².

Figure S38. Stress mean absolute error vs training points for Water 64, Set 1. Unit: meV/Å².
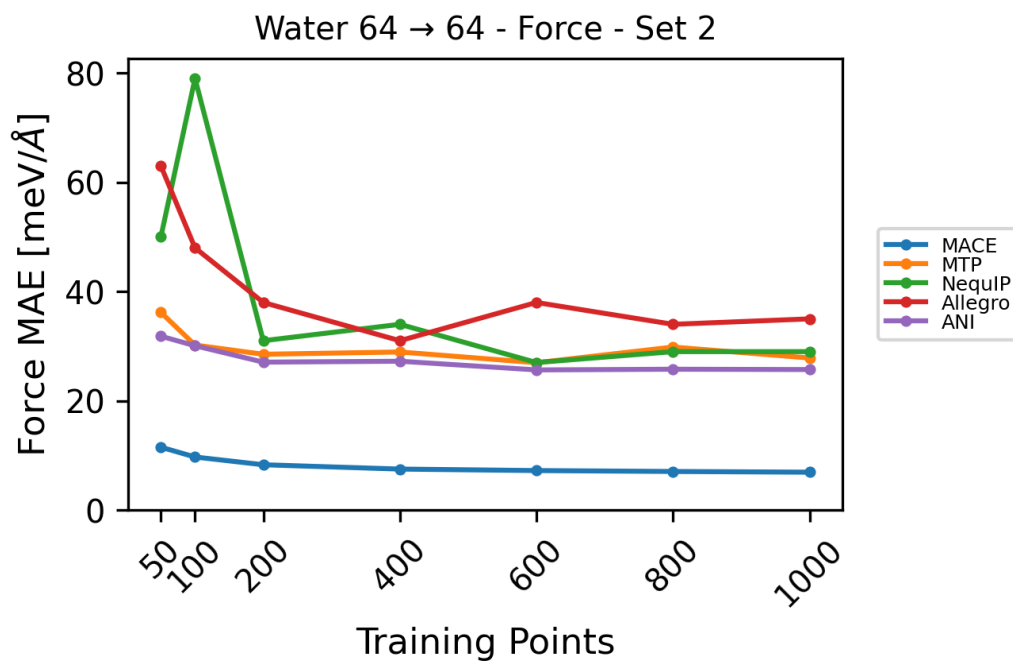
Figure S39. Energy mean absolute error vs training points for Water 64, Set 2. Unit: meV/atom.
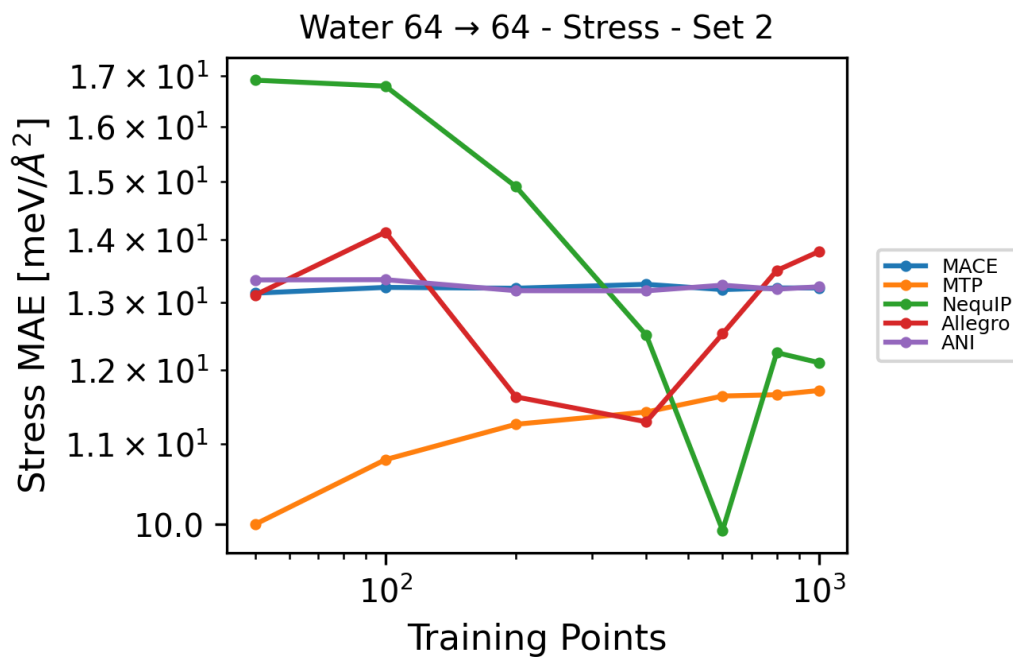
Figure S40. Energy mean absolute error vs training points for Water 64, Set 2. Unit: meV/atom.

Figure S41. Force mean absolute error vs training points for Water 64, Set 2. Unit: meV/Å.
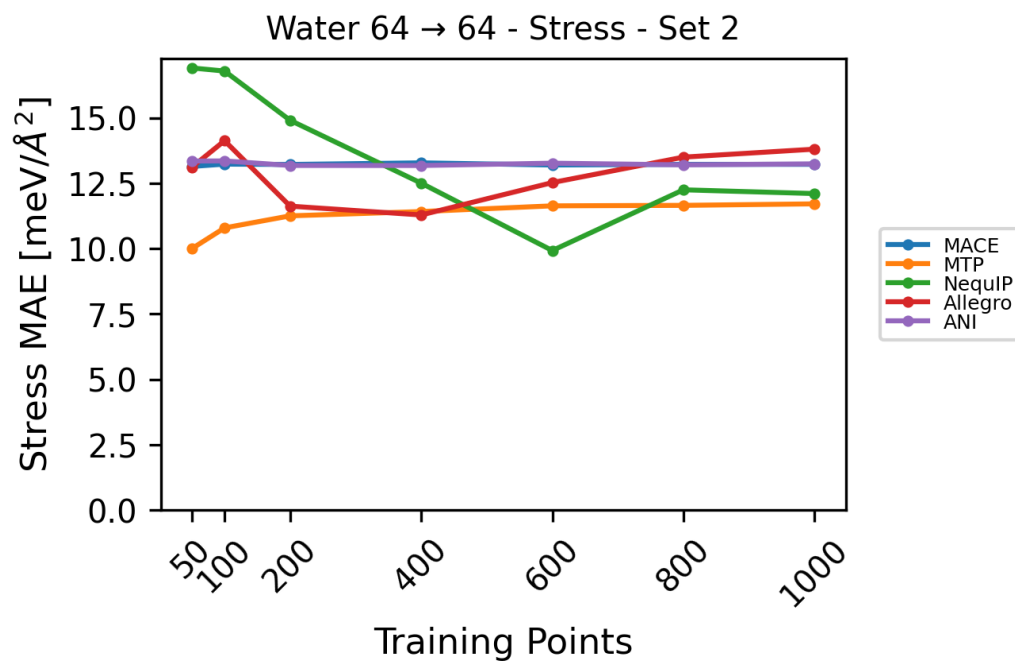
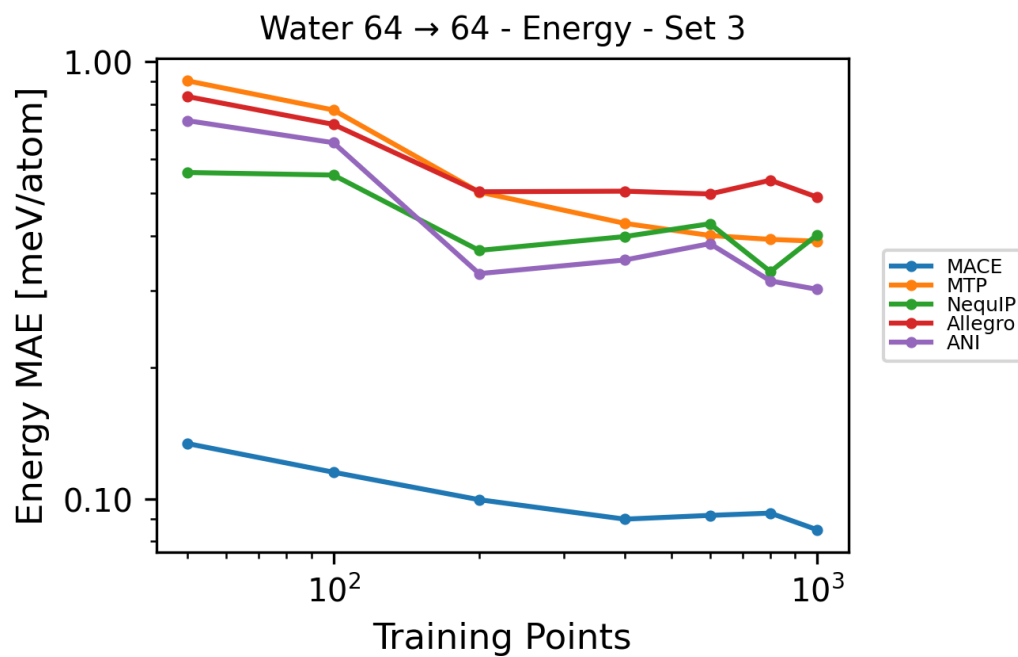**Figure S42.** Force mean absolute error vs training points for Water 64, Set 2. Unit: meV/Å.

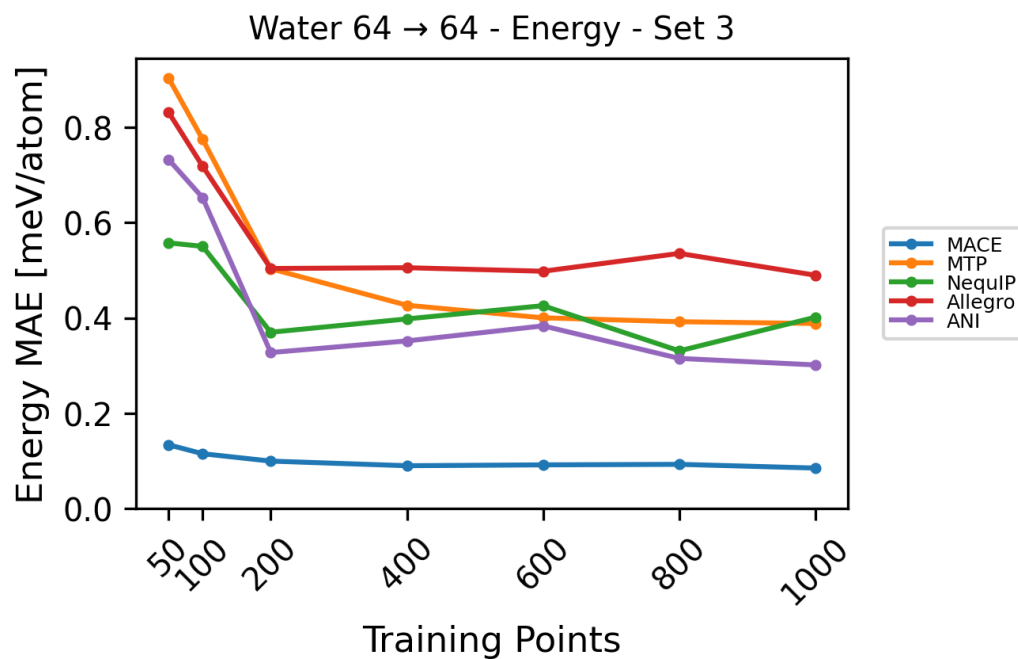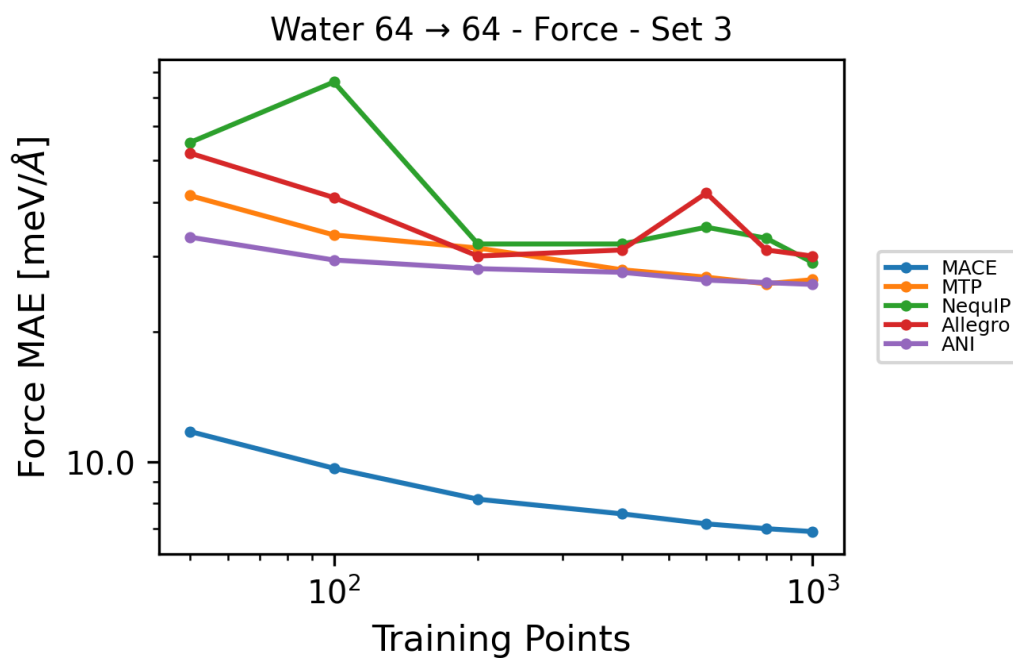**Figure S43.** Stress mean absolute error vs training points for Water 64, Set 2. Unit: meV/Å².

Figure S44. Stress mean absolute error vs training points for Water 64, Set 2. Unit: meV/Å².
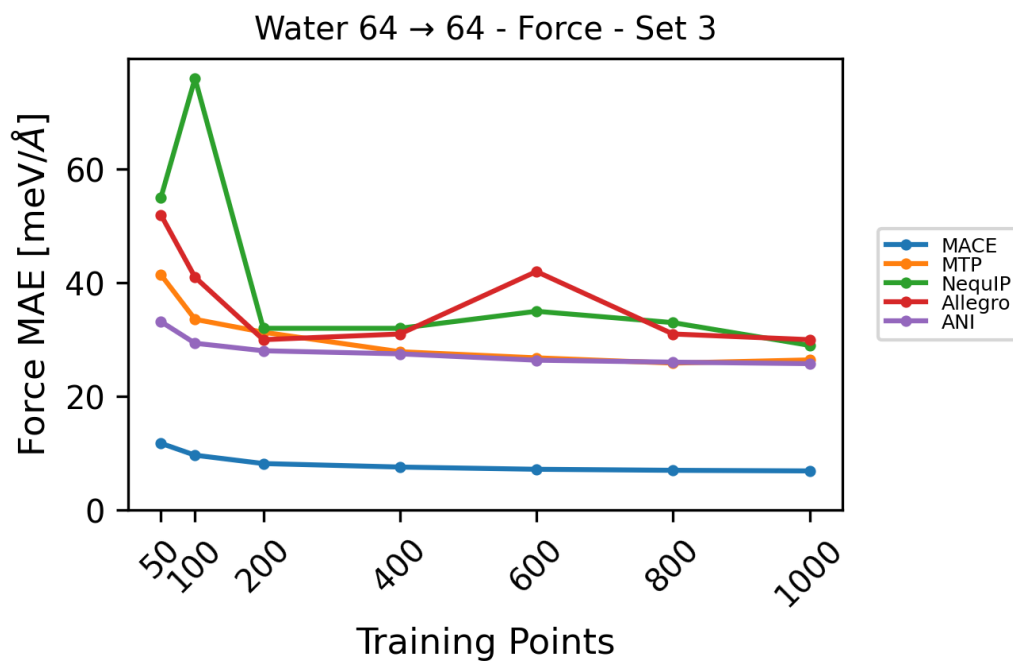
Figure S45. Energy mean absolute error vs training points for Water 64, Set 3. Unit: meV/atom.
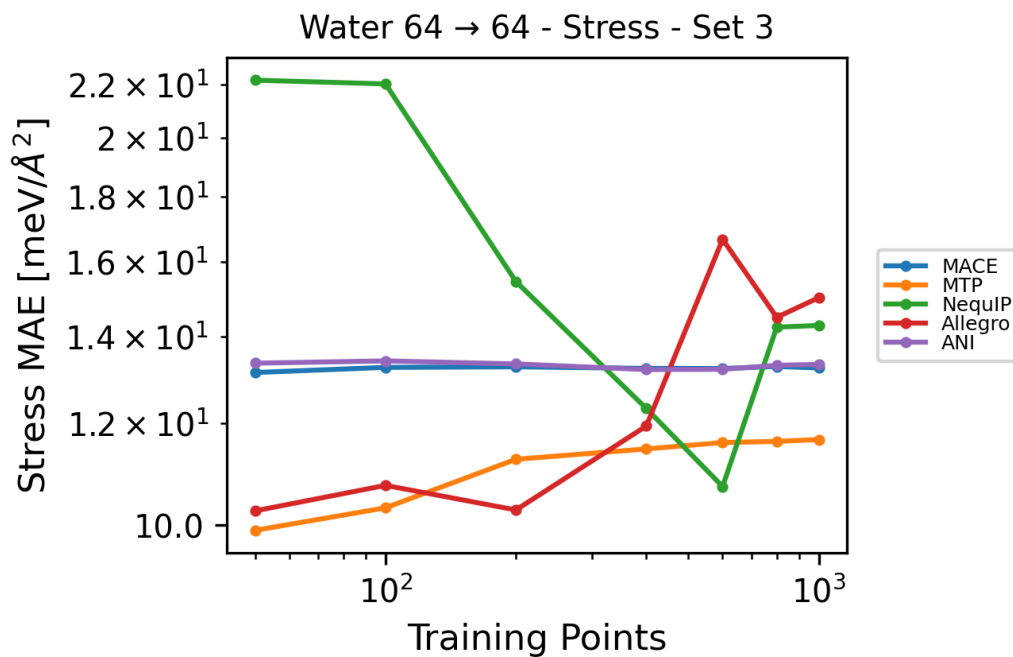
Figure S46. Energy mean absolute error vs training points for Water 64, Set 3. Unit: meV/atom.
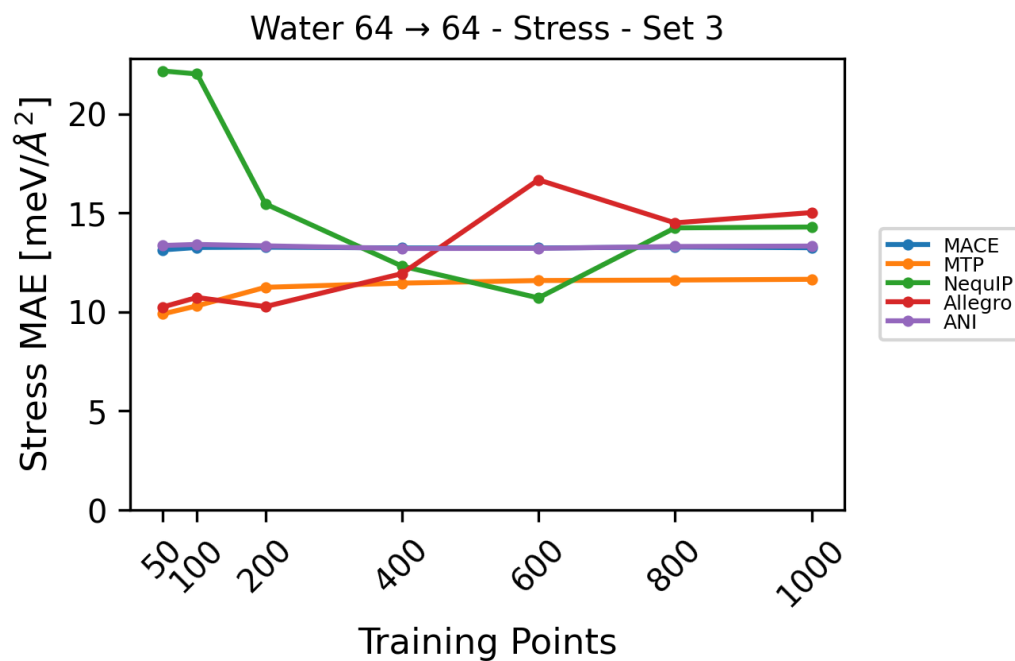
Figure S47. Force mean absolute error vs training points for Water 64, Set 3. Unit: meV/Å.
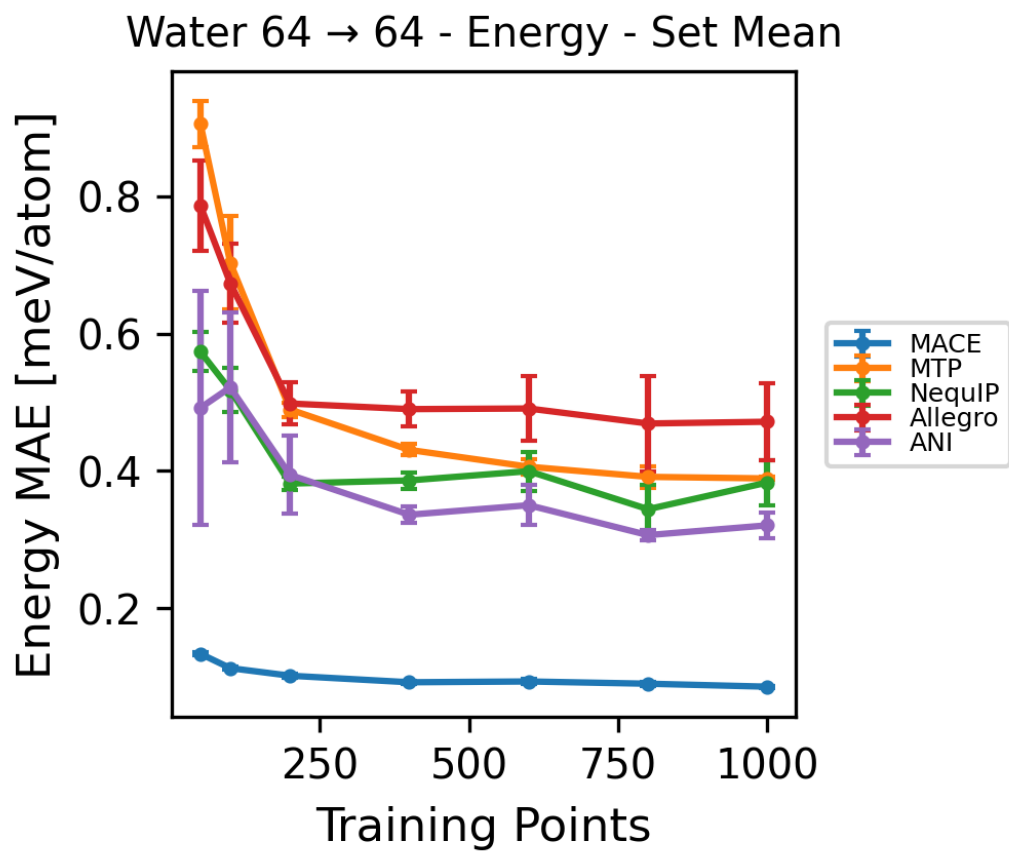
Figure S48. Force mean absolute error vs training points for Water 64, Set 3. Unit: meV/Å.

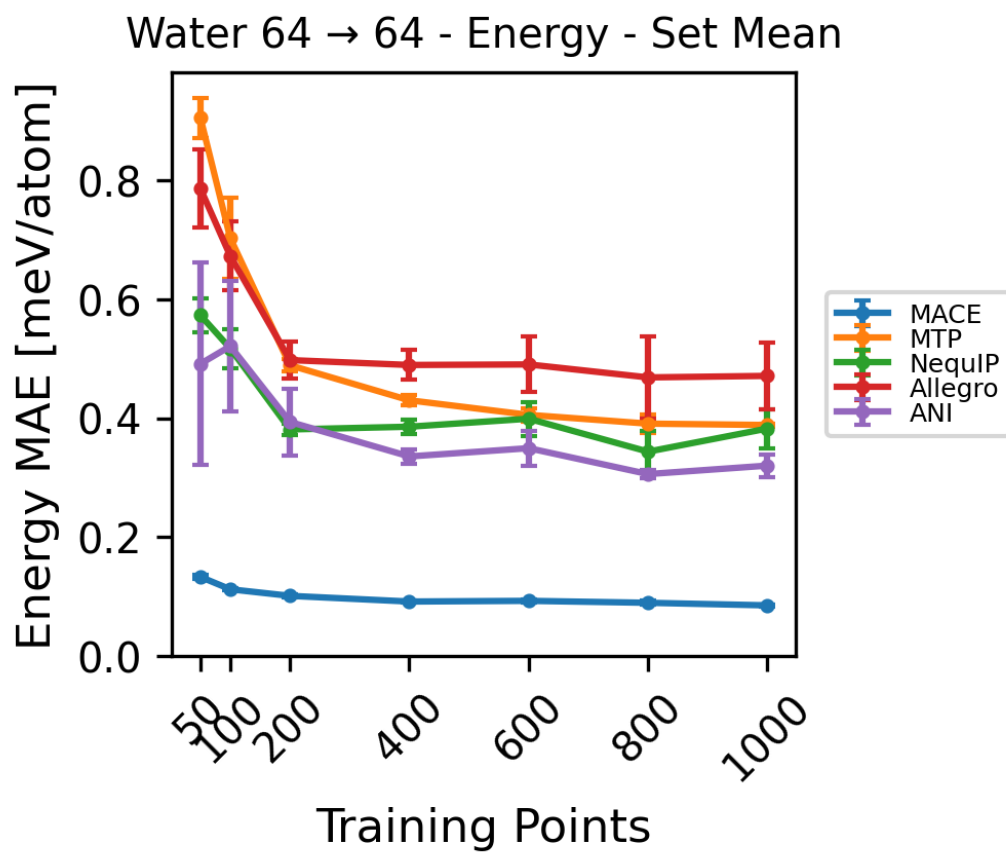**Figure S49.** Stress mean absolute error vs training points for Water 64, Set 3. Unit: meV/Å².

Figure S50. Stress mean absolute error vs training points for Water 64, Set 3. Unit: meV/Å².
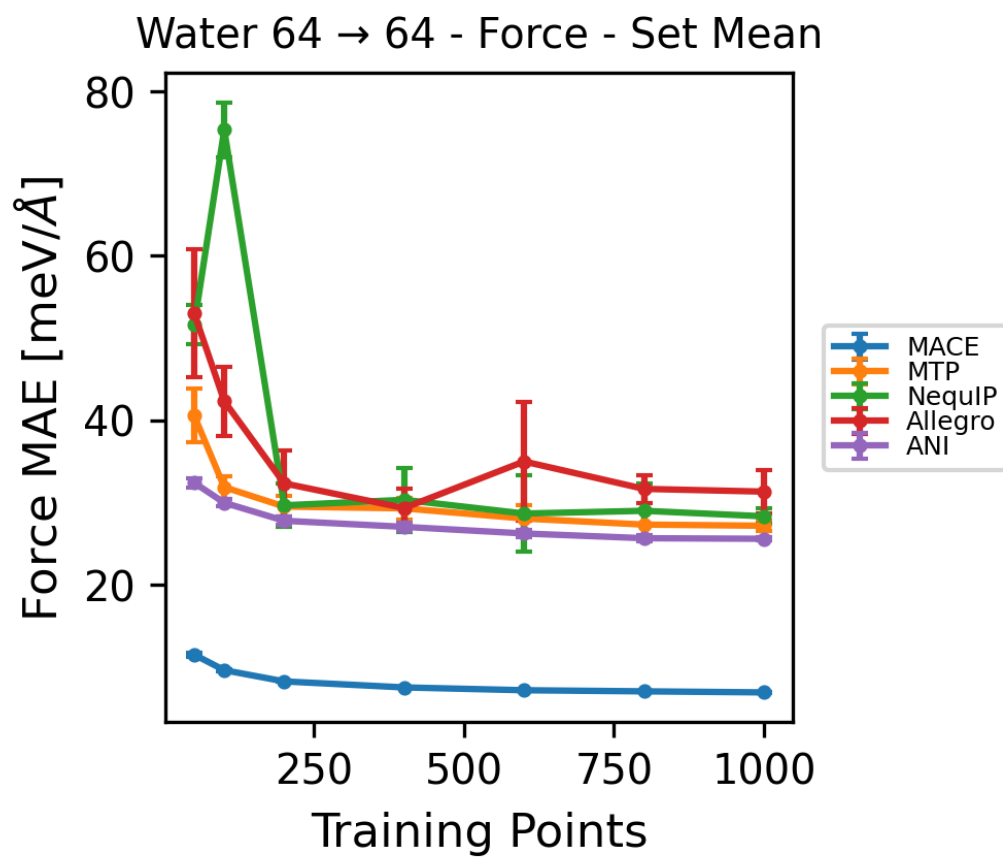
Figure S51. Energy mean absolute error vs training points for Water 64, Set mean. Unit: meV/atom.
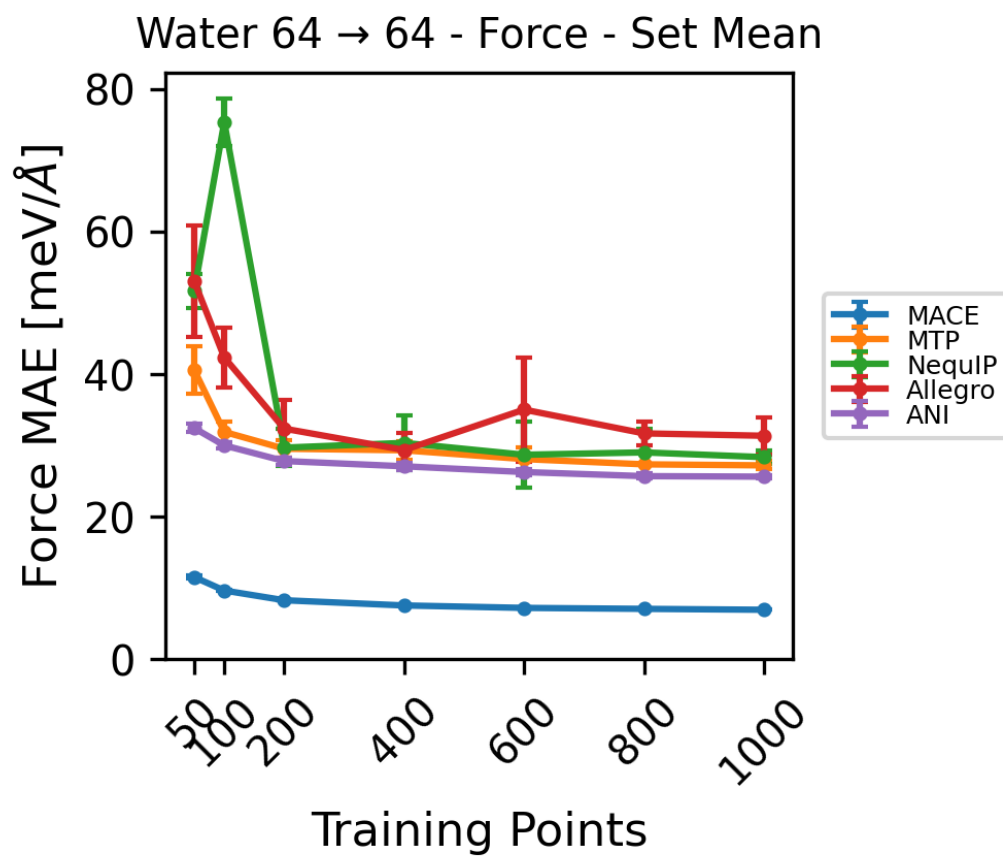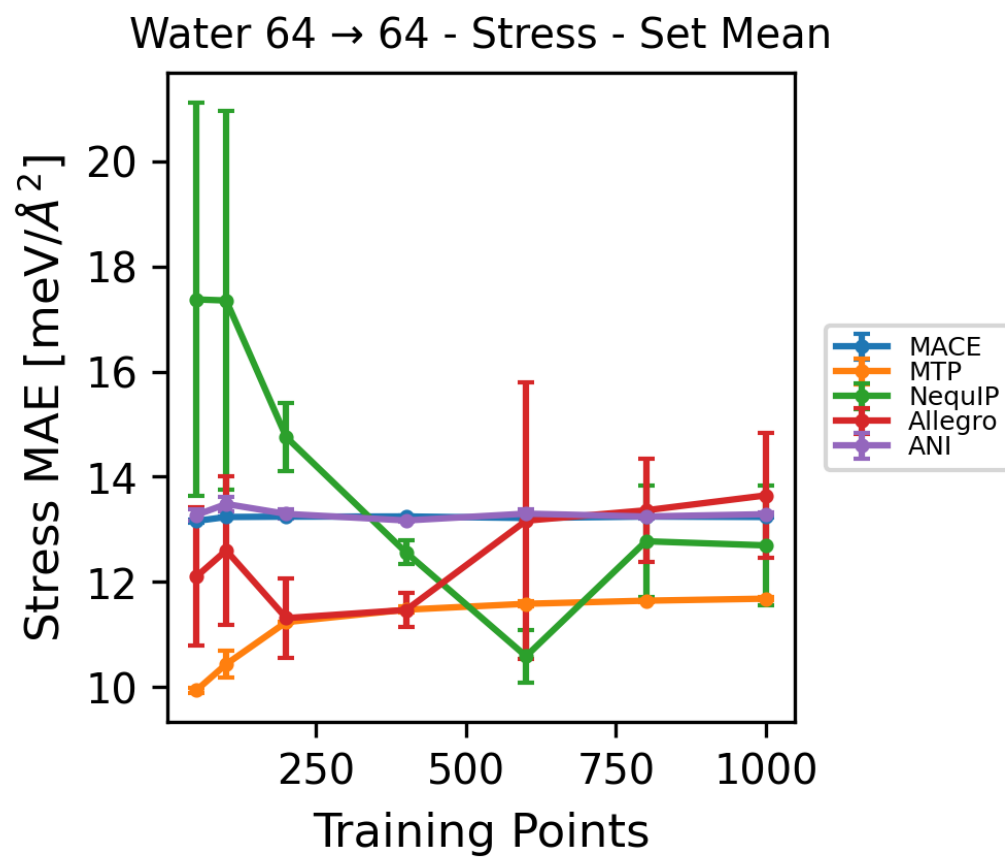
Figure S52. Energy mean absolute error vs training points for Water 64, Set mean. Unit: meV/atom.
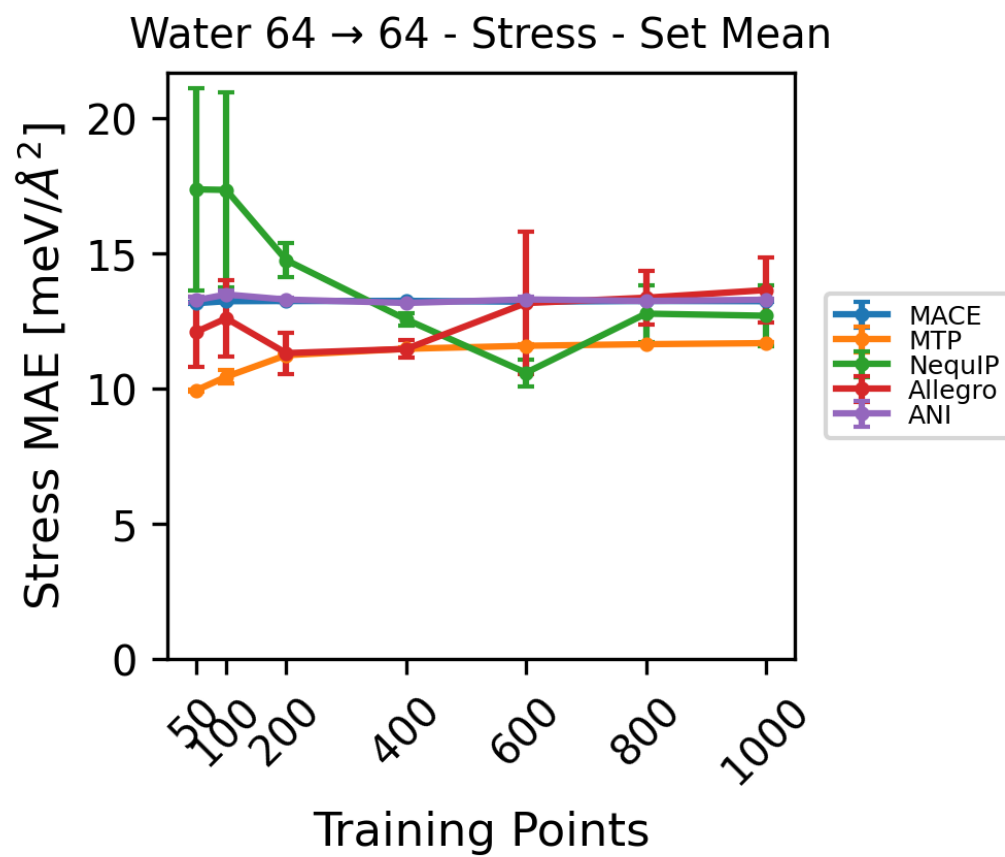
Figure S53. Force mean absolute error vs training points for Water 64, Set mean. Unit: meV/Å.

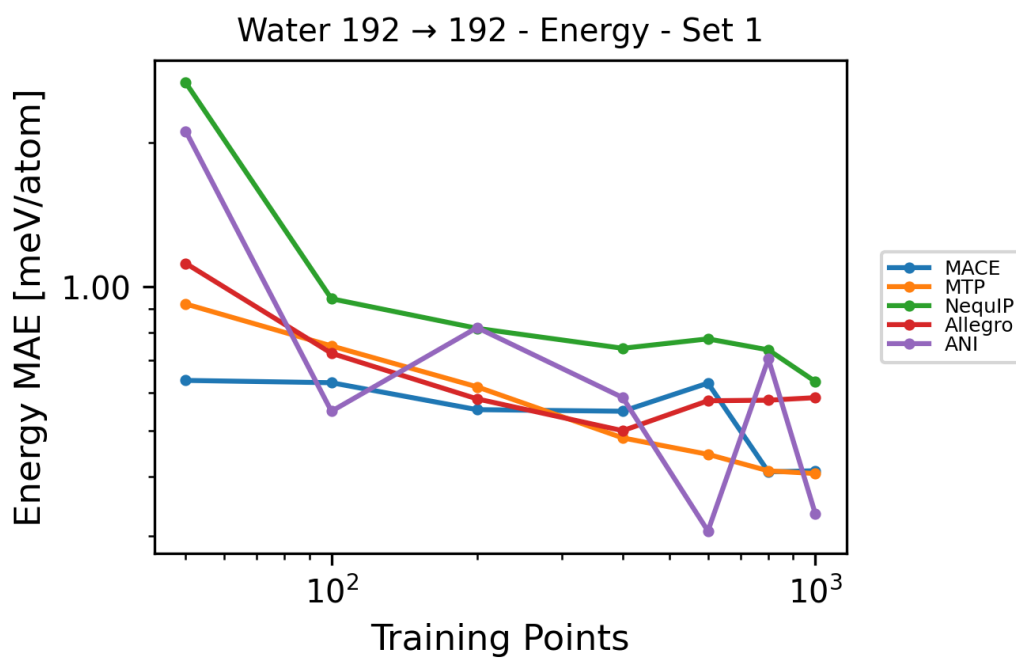**Figure S54.** Force mean absolute error vs training points for Water 64, Set mean. Unit: meV/Å.

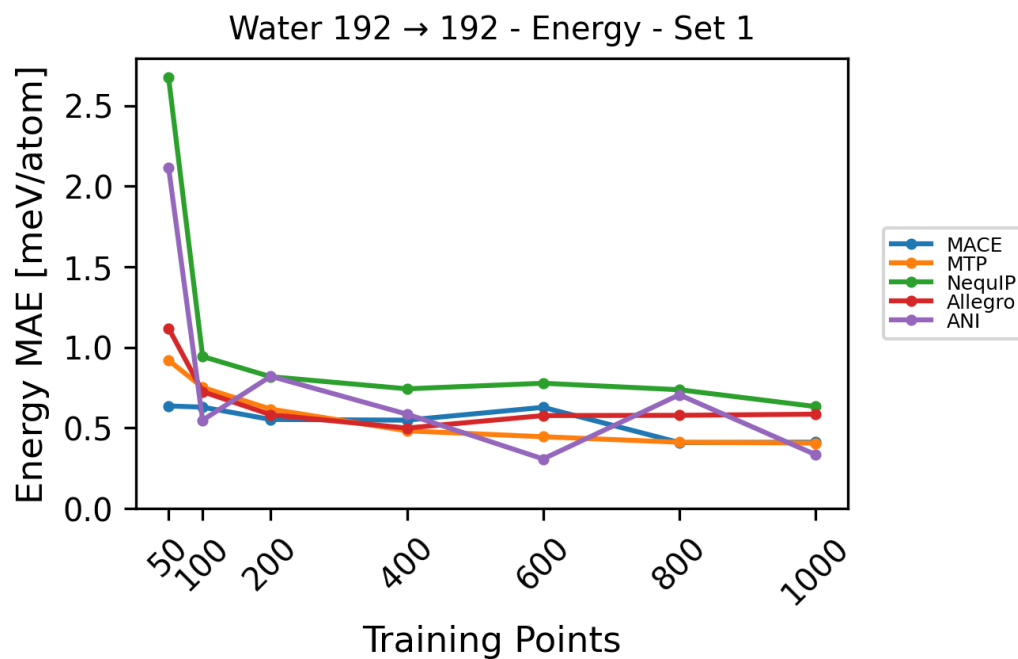**Figure S55.** Stress mean absolute error vs training points for Water 64, Set mean. Unit: meV/Å².

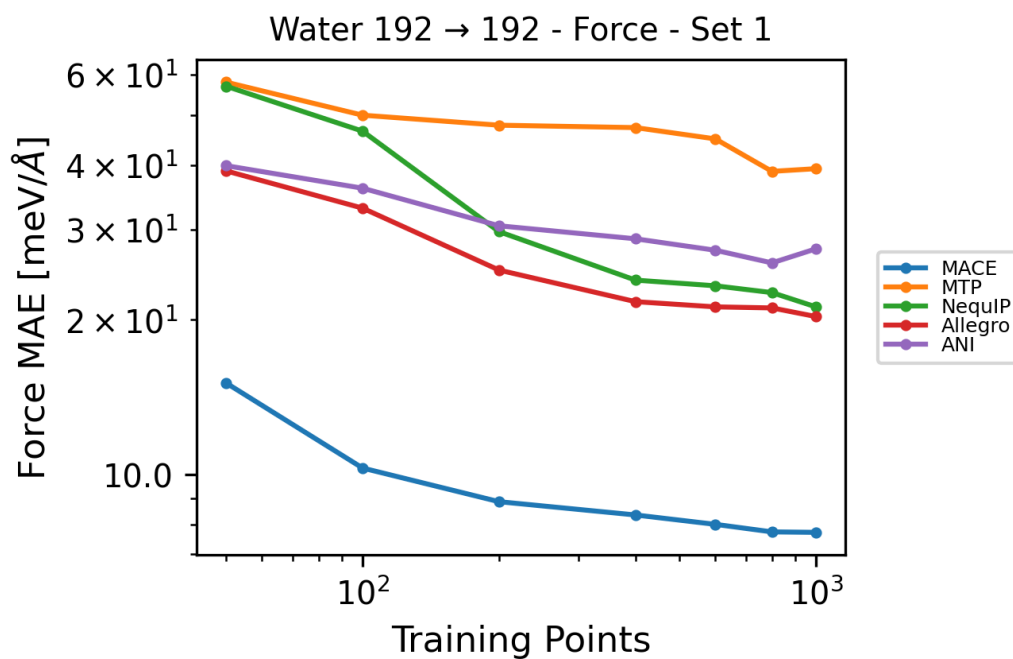**Figure S56.** Stress mean absolute error vs training points for Water 64, Set mean. Unit: meV/Å².

Water 192

Figure S57. Energy mean absolute error vs training points for Water 192, Set 1. Unit: meV/atom.
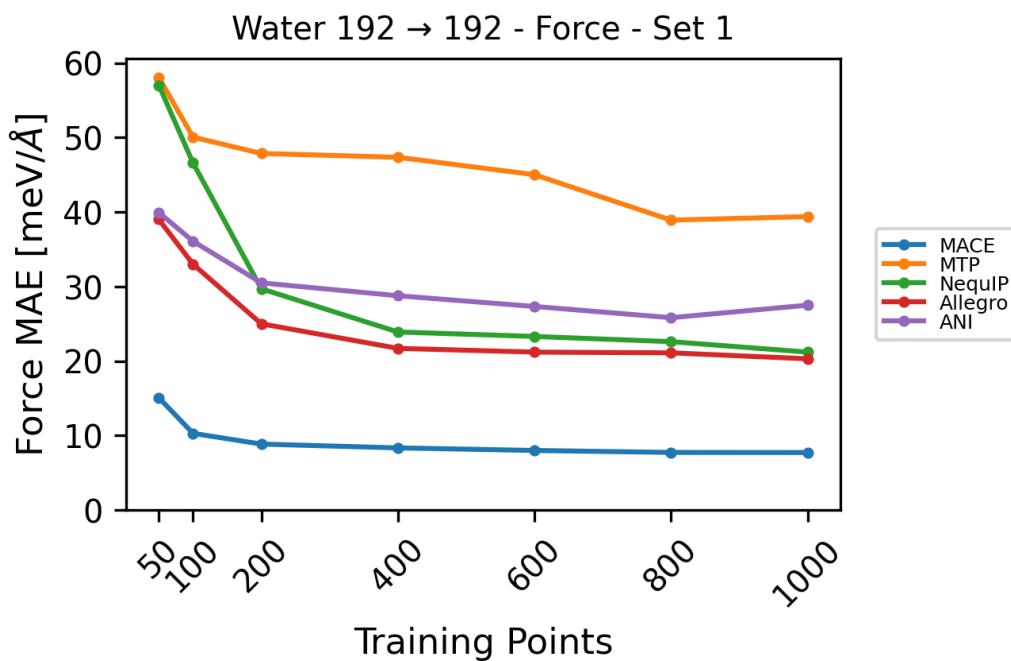
Figure S58. Energy mean absolute error vs training points for Water 192, Set 1. Unit: meV/atom.
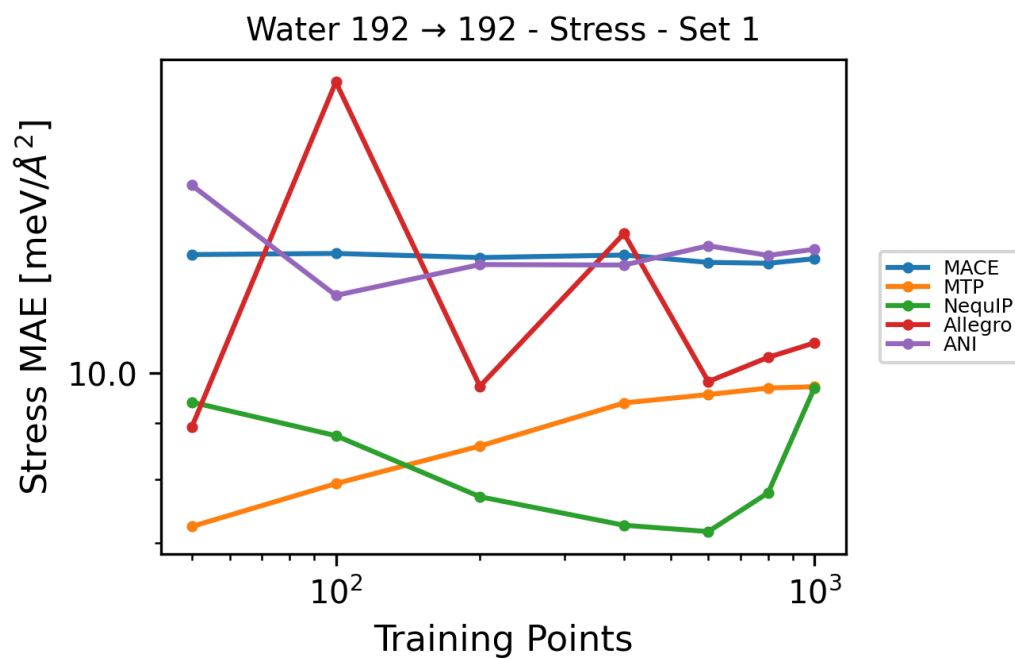
Figure S59. Force mean absolute error vs training points for Water 192, Set 1. Unit: meV/Å.
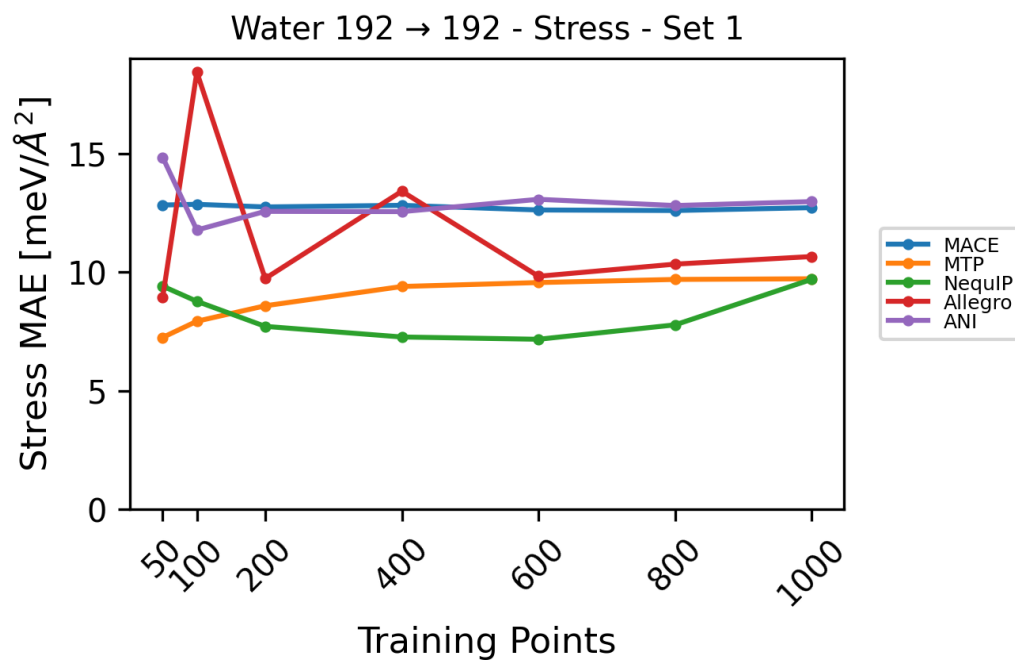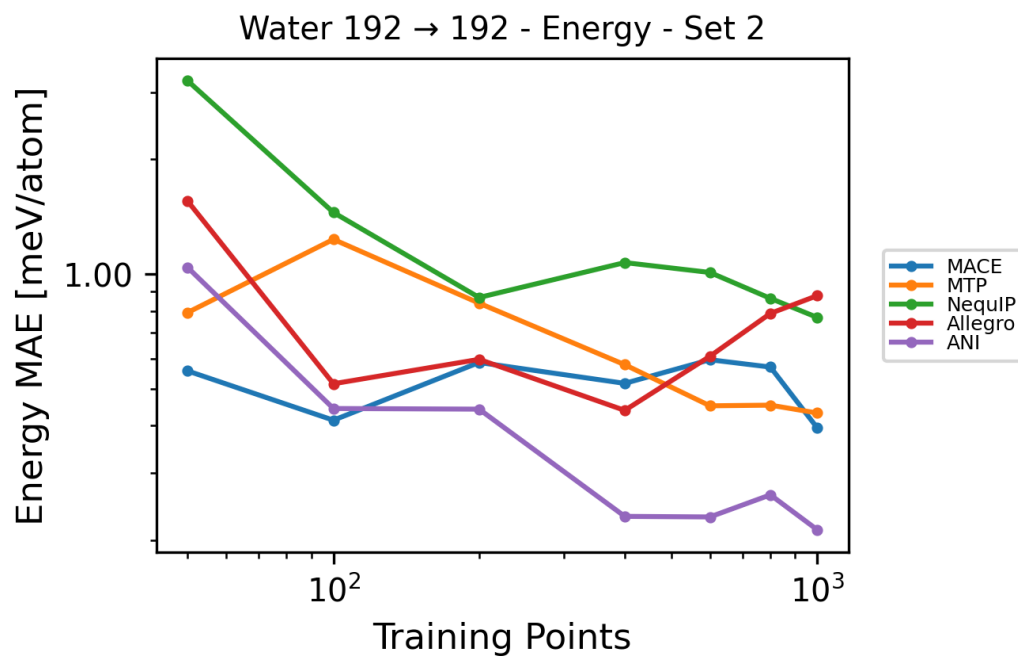
Figure S60. Force mean absolute error vs training points for Water 192, Set 1. Unit: meV/Å.
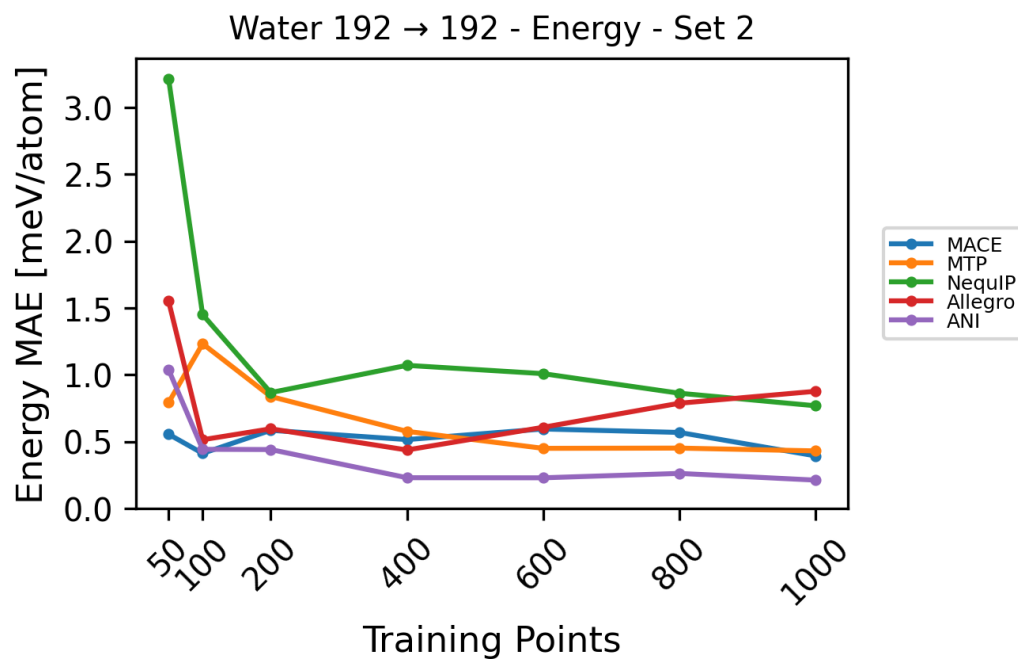
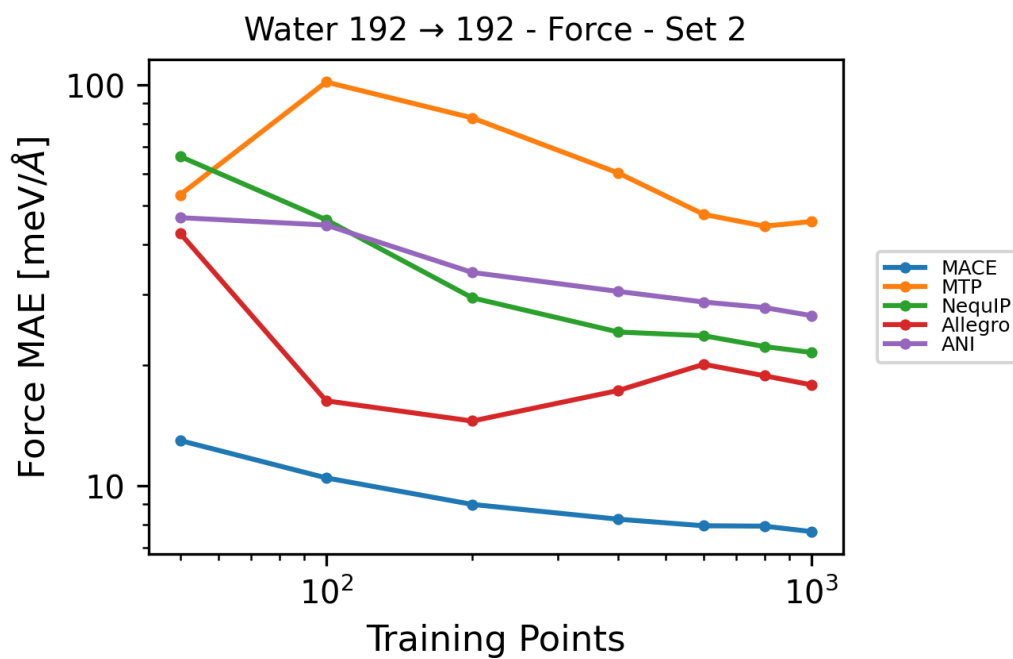**Figure S61.** Stress mean absolute error vs training points for Water 192, Set 1. Unit: meV/Å².

Figure S62. Stress mean absolute error vs training points for Water 192, Set 1. Unit: meV/Å².
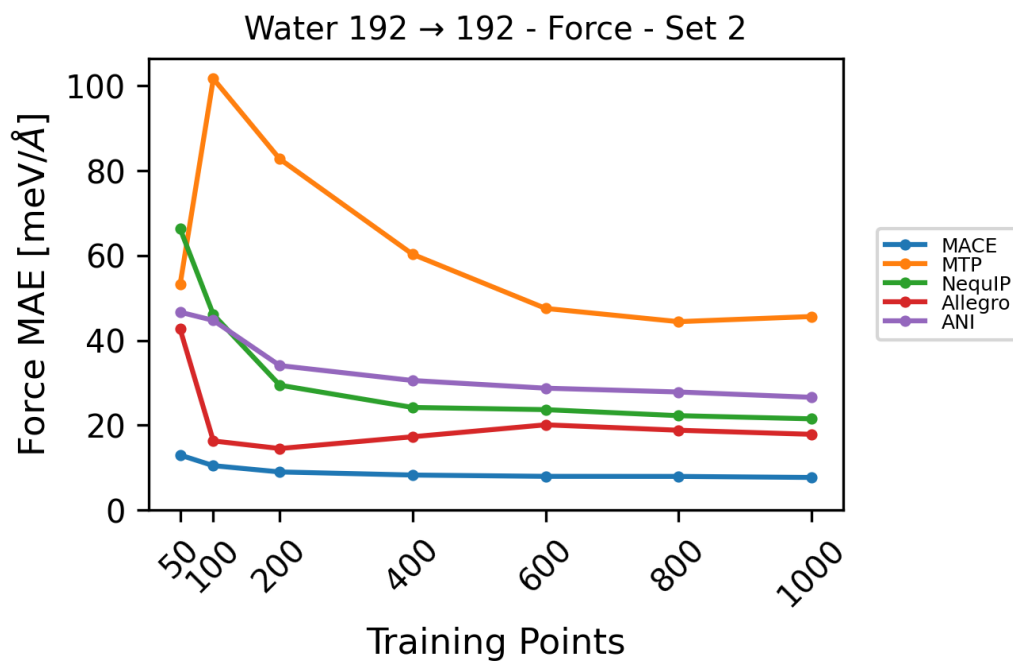
Figure S63. Energy mean absolute error vs training points for Water 192, Set 2. Unit: meV/atom.
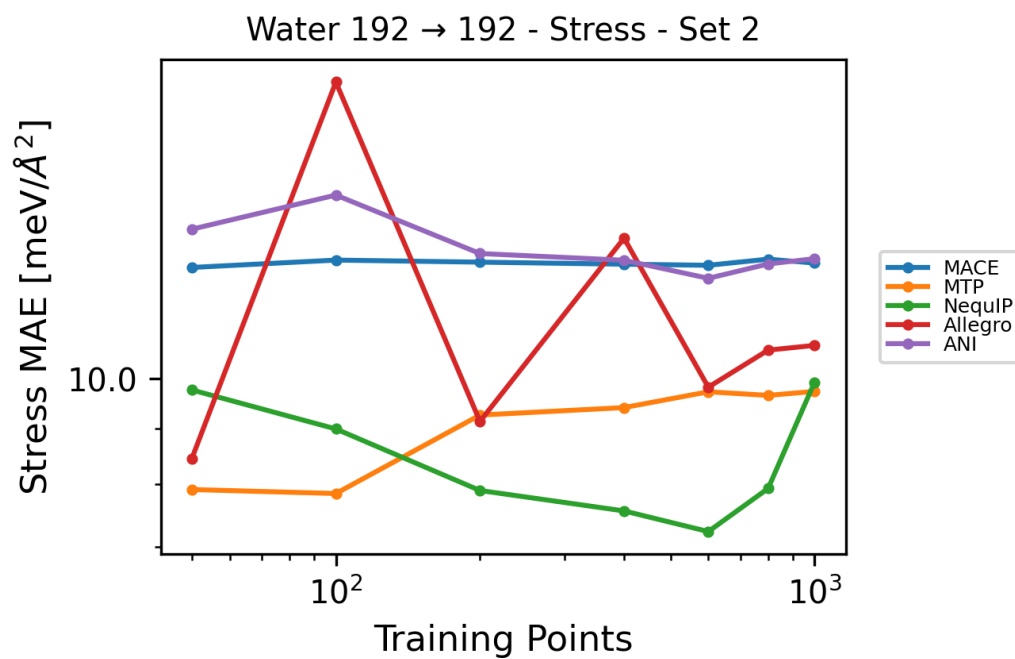
Figure S64. Energy mean absolute error vs training points for Water 192, Set 2. Unit: meV/atom.

Figure S65. Force mean absolute error vs training points for Water 192, Set 2. Unit: meV/Å.
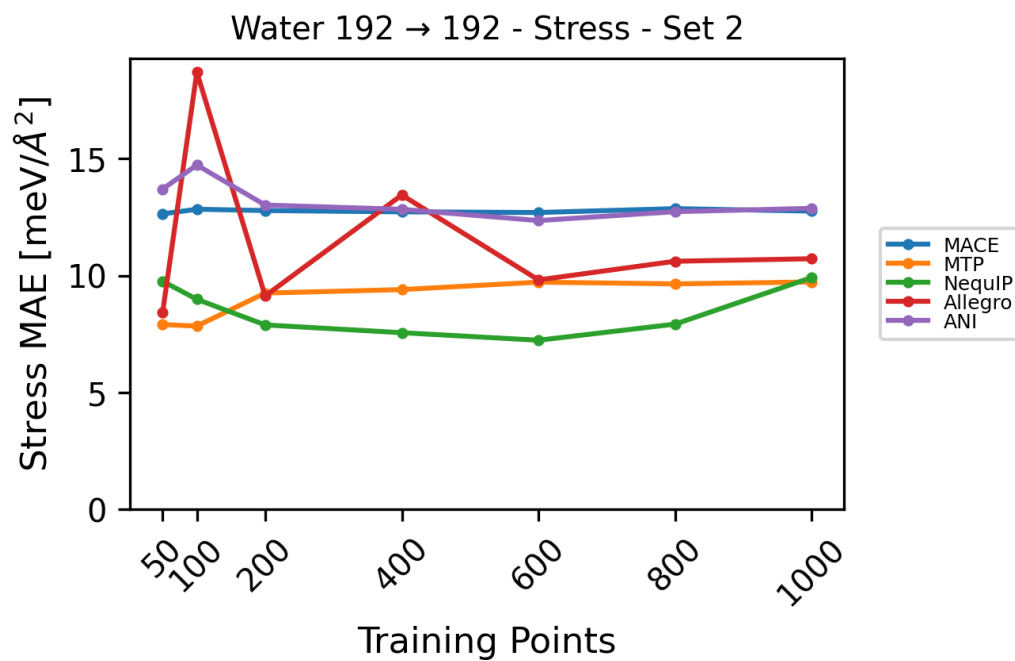
Figure S66. Force mean absolute error vs training points for Water 192, Set 2. Unit: meV/Å.
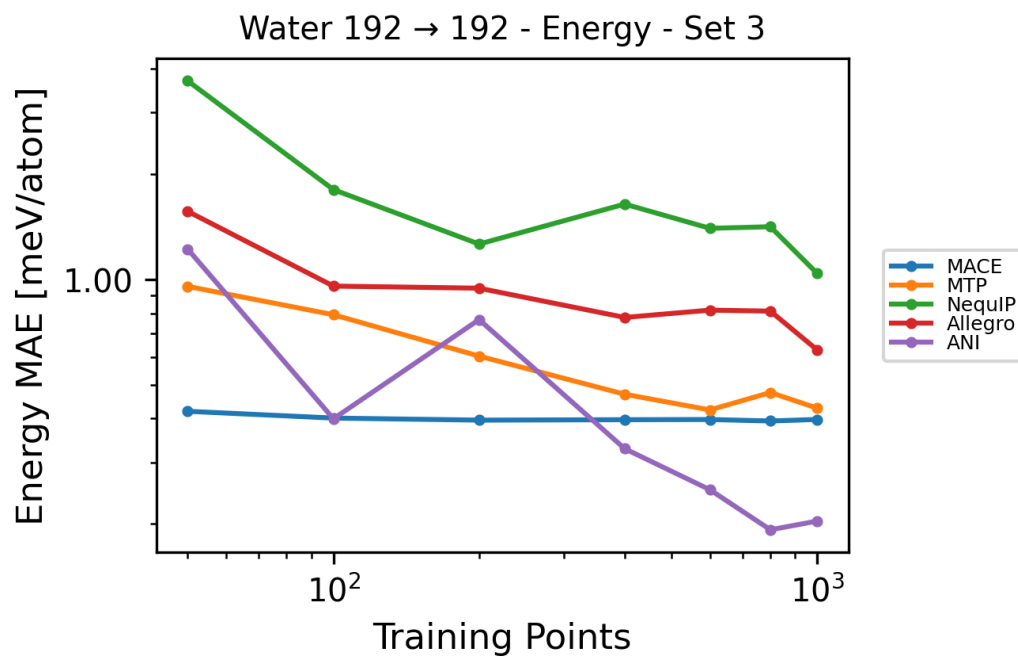
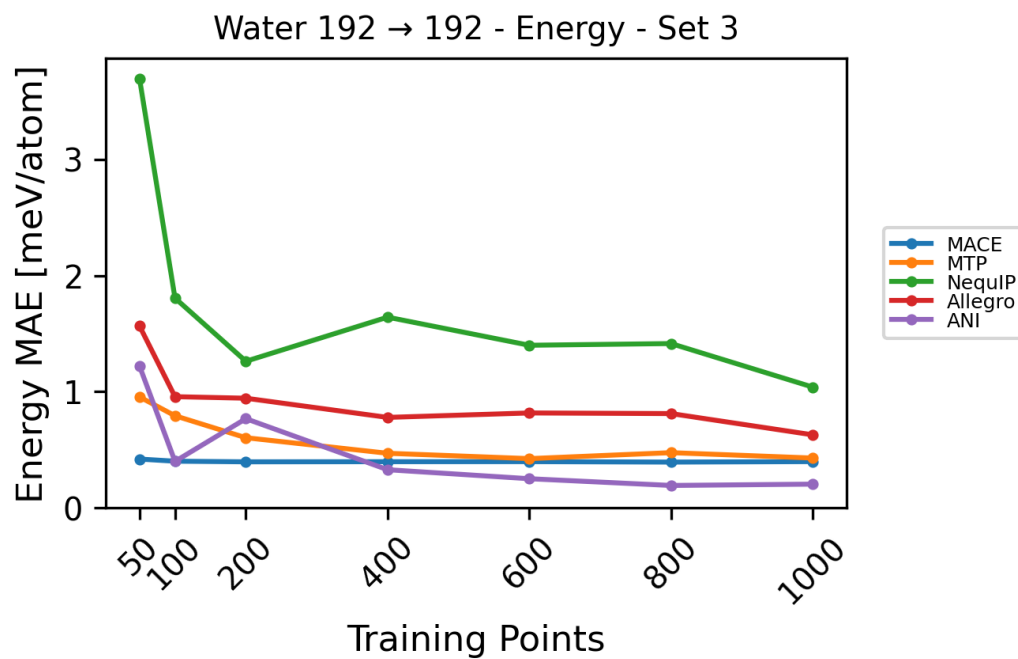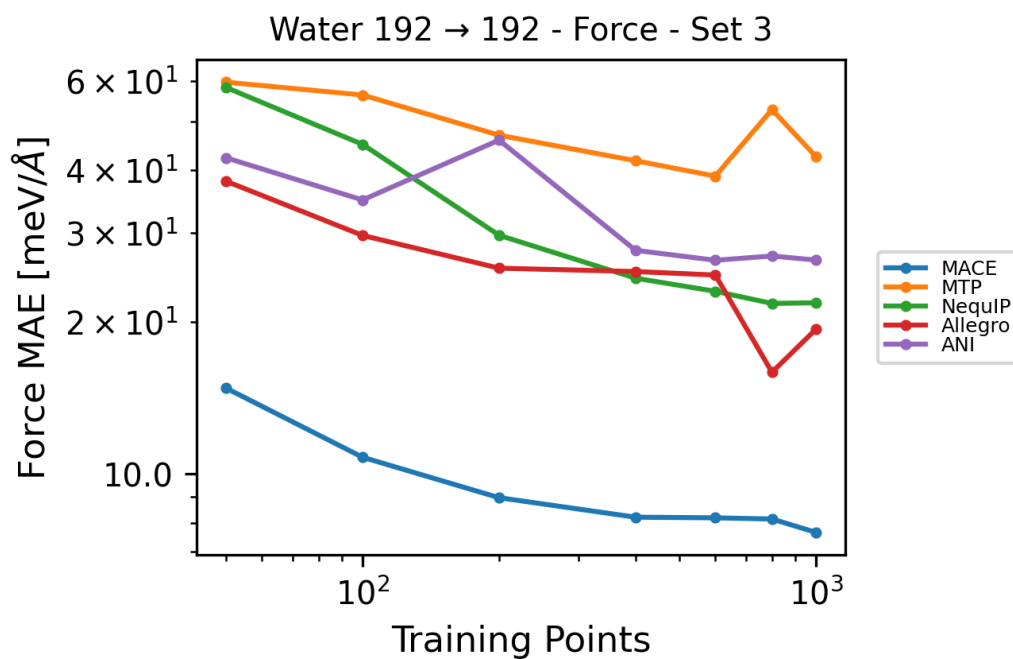**Figure S67.** Stress mean absolute error vs training points for Water 192, Set 2. Unit: meV/Å².

Figure S68. Stress mean absolute error vs training points for Water 192, Set 2. Unit: meV/Å².
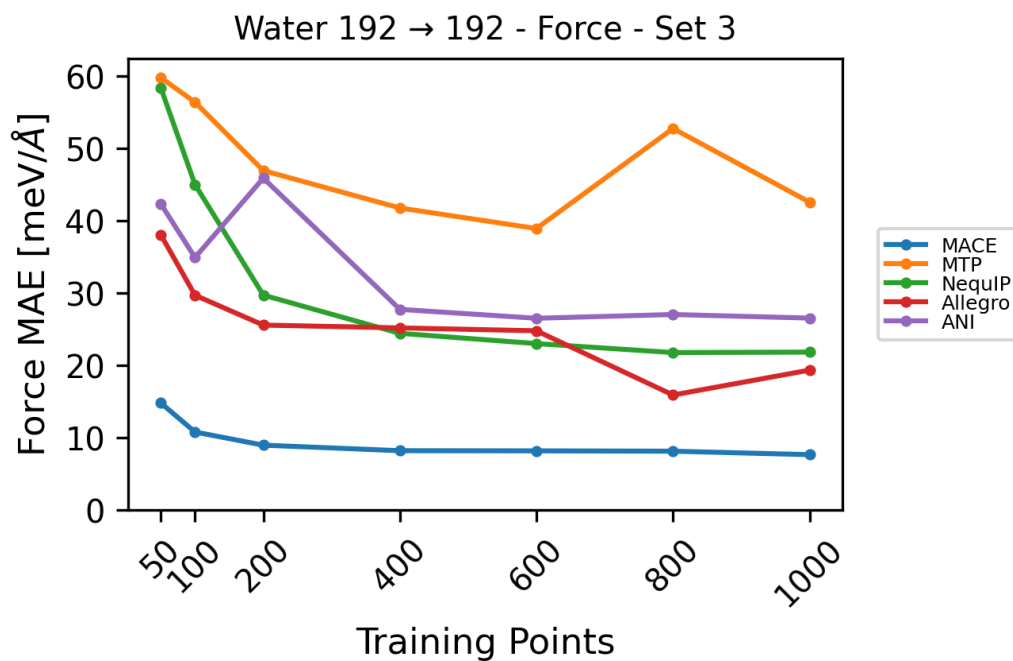
Figure S69. Energy mean absolute error vs training points for Water 192, Set 3. Unit: meV/atom.
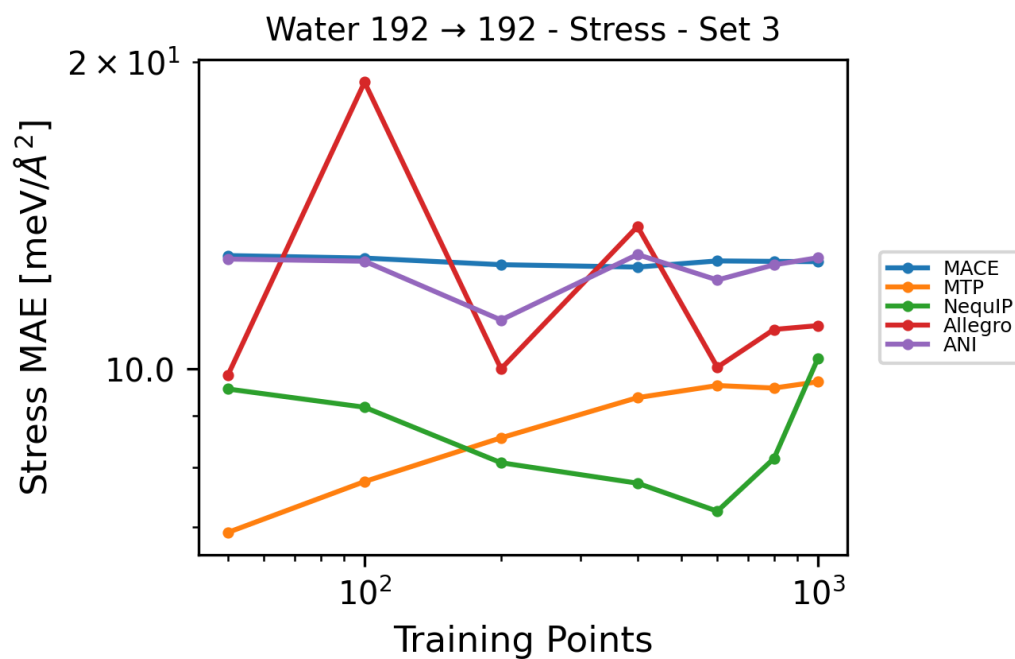
Figure S70. Energy mean absolute error vs training points for Water 192, Set 3. Unit: meV/atom.
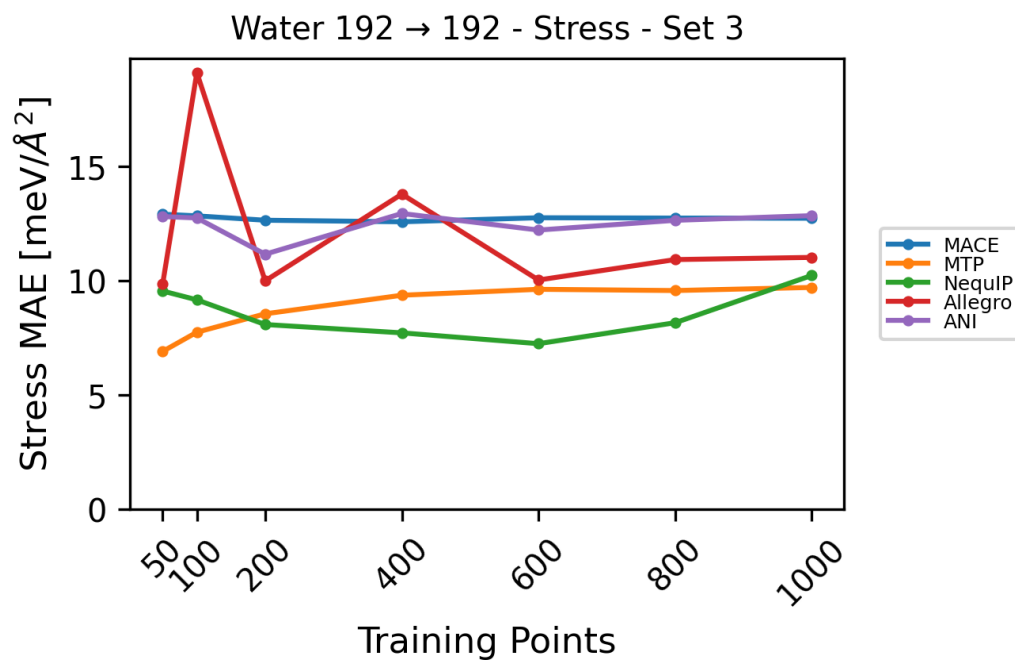
Figure S71. Force mean absolute error vs training points for Water 192, Set 3. Unit: meV/Å.
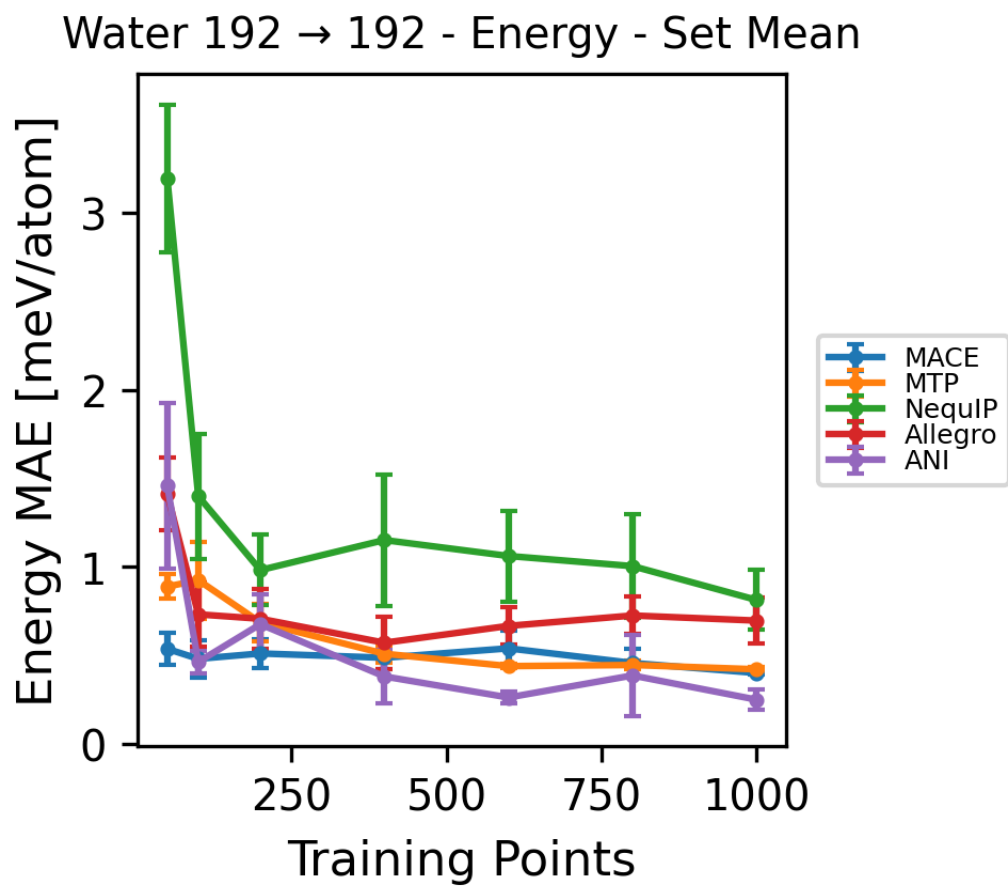
Figure S72. Force mean absolute error vs training points for Water 192, Set 3. Unit: meV/Å.

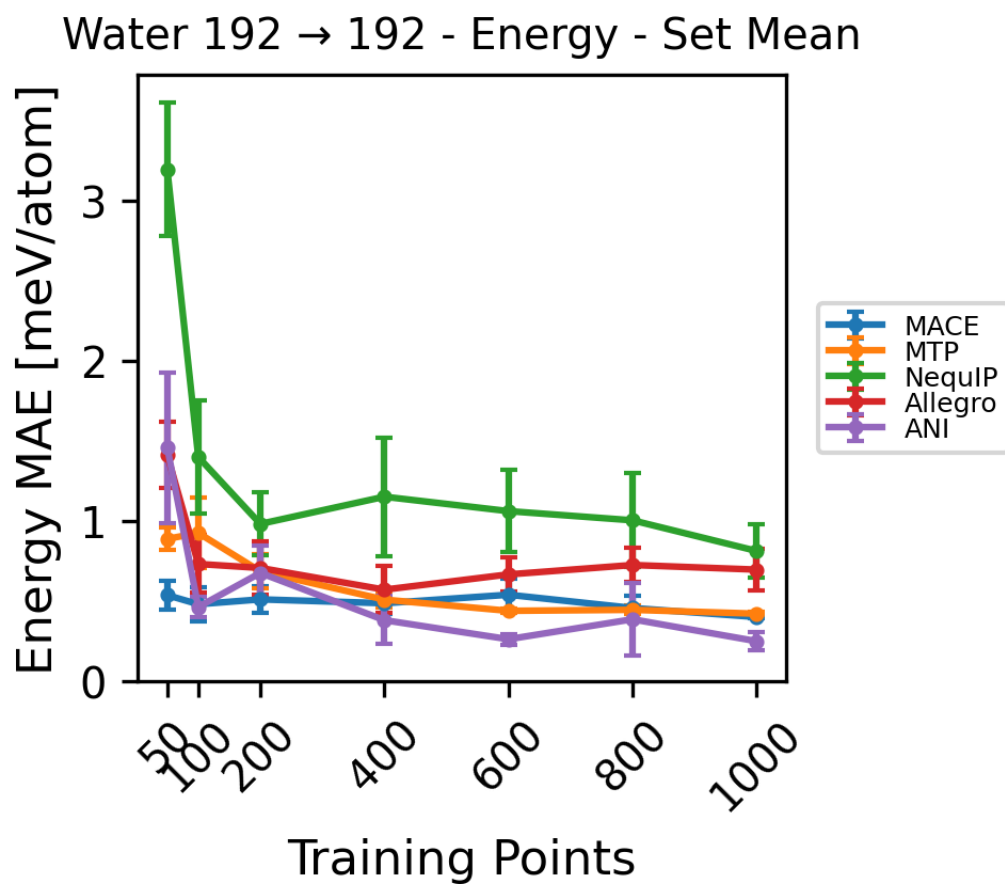**Figure S73.** Stress mean absolute error vs training points for Water 192, Set 3. Unit: meV/Å².

Figure S74. Stress mean absolute error vs training points for Water 192, Set 3. Unit: meV/Å².
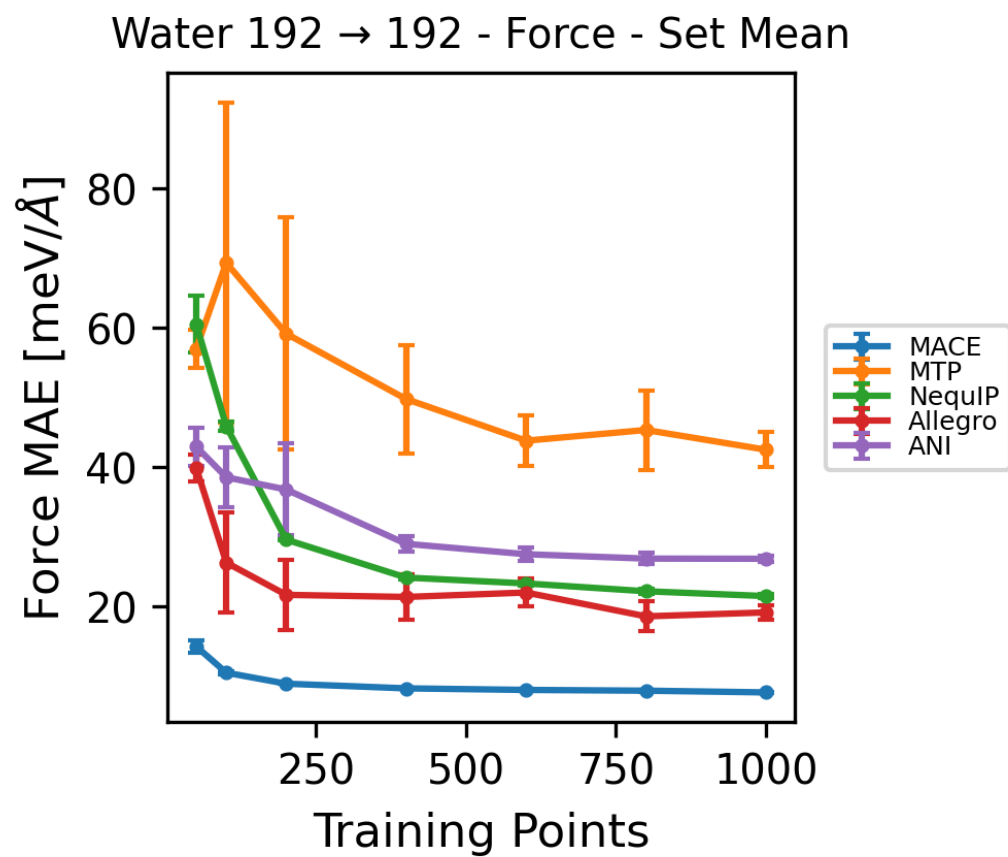
Figure S75. Energy mean absolute error vs training points for Water 192, Set mean. Unit: meV/atom.
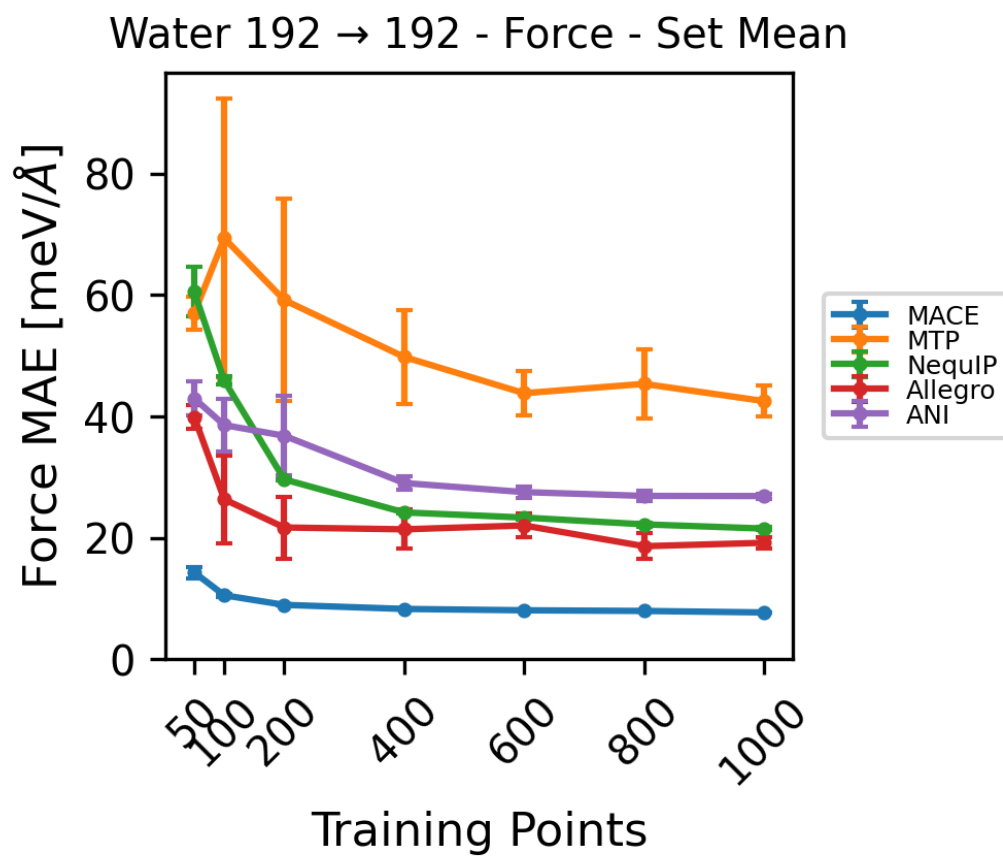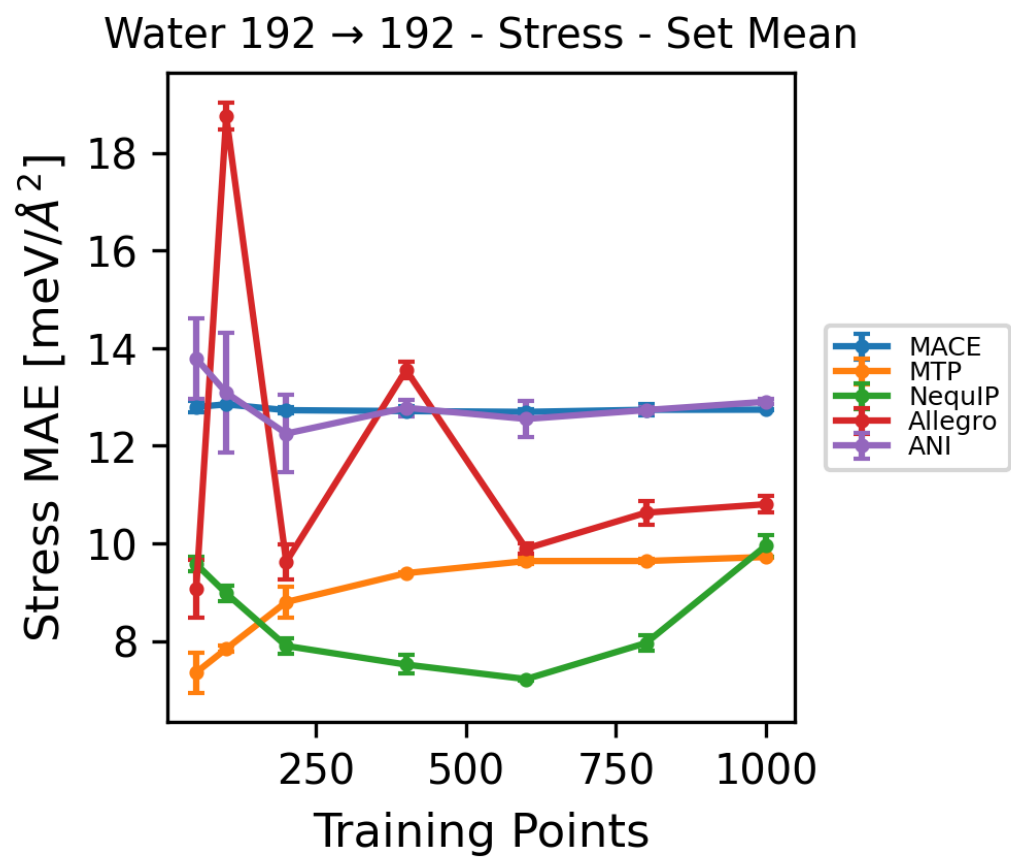
Figure S76. Energy mean absolute error vs training points for Water 192, Set mean. Unit: meV/atom.
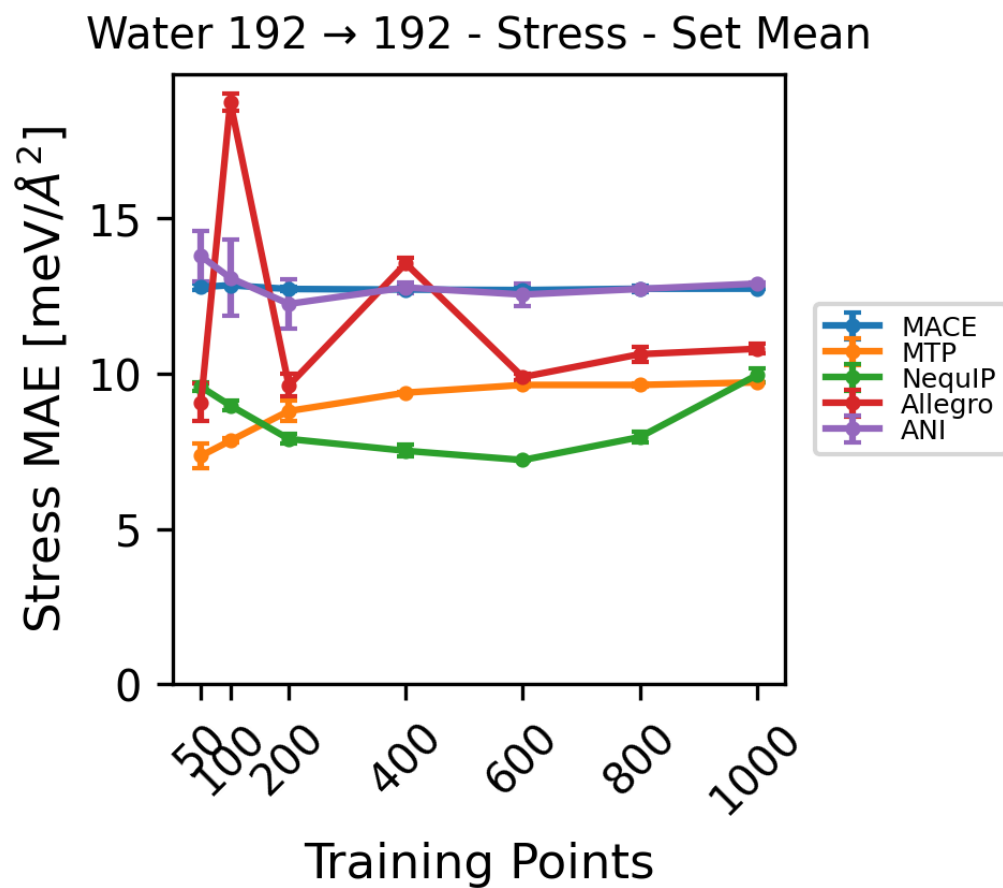
Figure S77. Force mean absolute error vs training points for Water 192, Set mean. Unit: meV/Å.

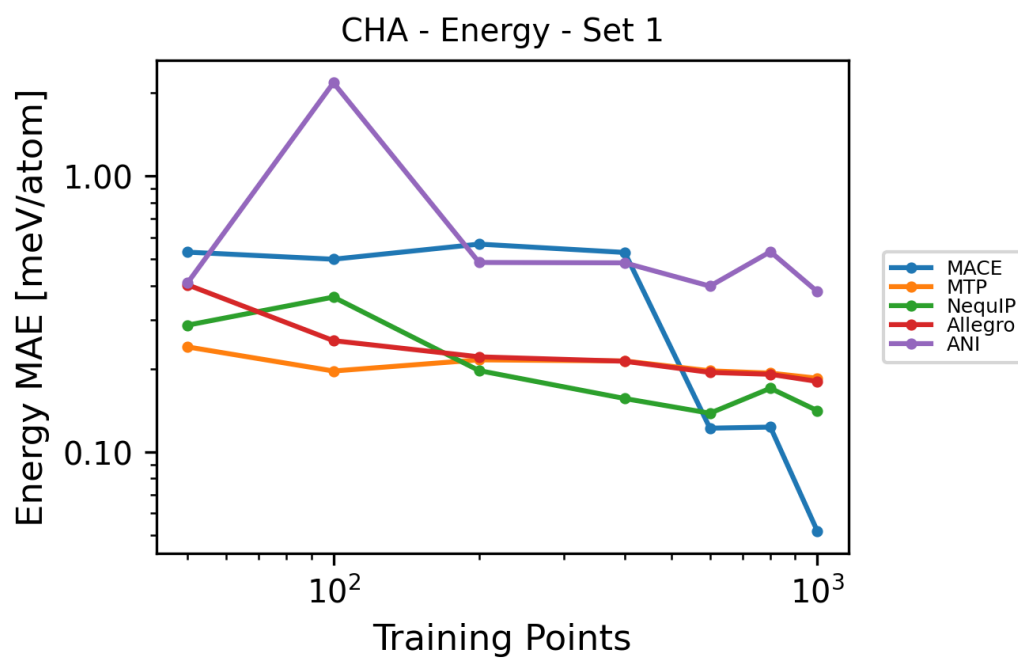**Figure S78.** Force mean absolute error vs training points for Water 192, Set mean. Unit: meV/Å.

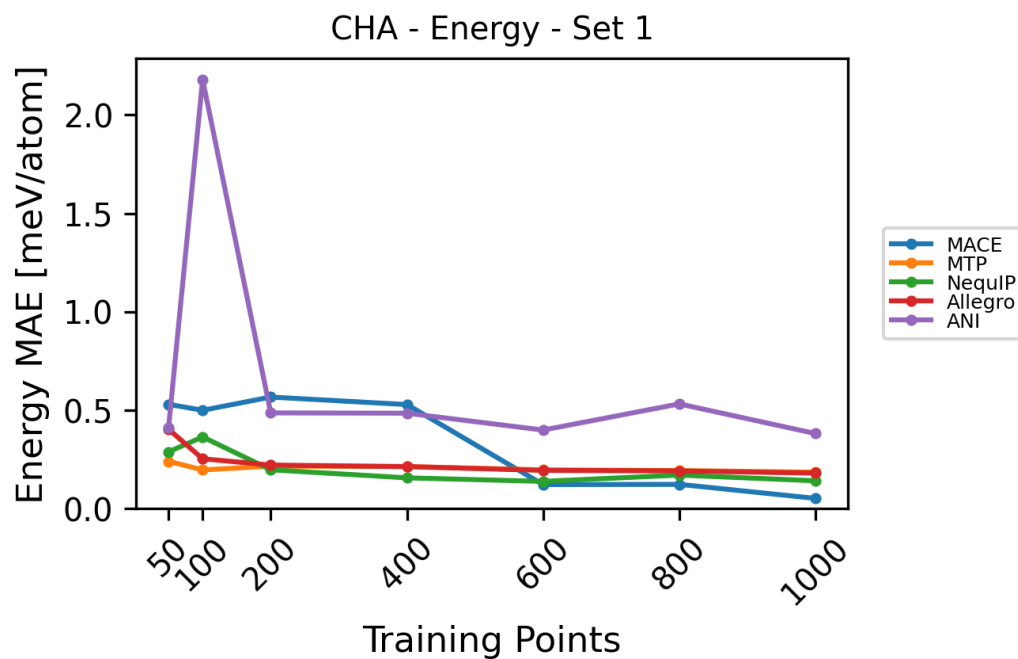**Figure S79.** Stress mean absolute error vs training points for Water 192, Set mean. Unit: meV/Å².

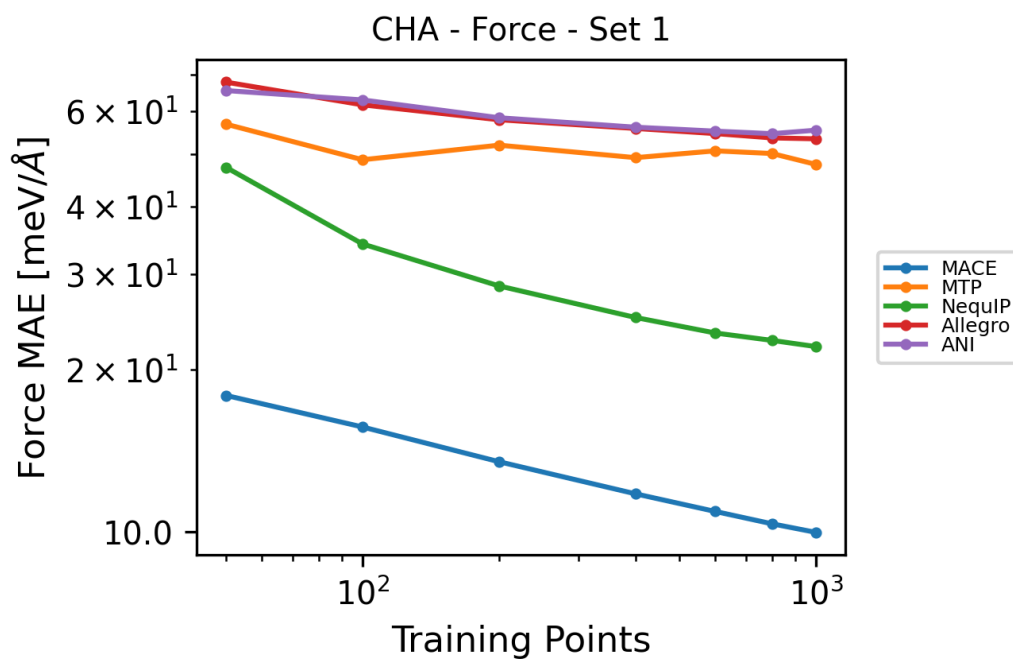**Figure S80.** Stress mean absolute error vs training points for Water 192, Set mean. Unit: meV/Å².

CHA

Figure S81. Energy mean absolute error vs training points for CHA, Set 1. Unit: meV/atom.
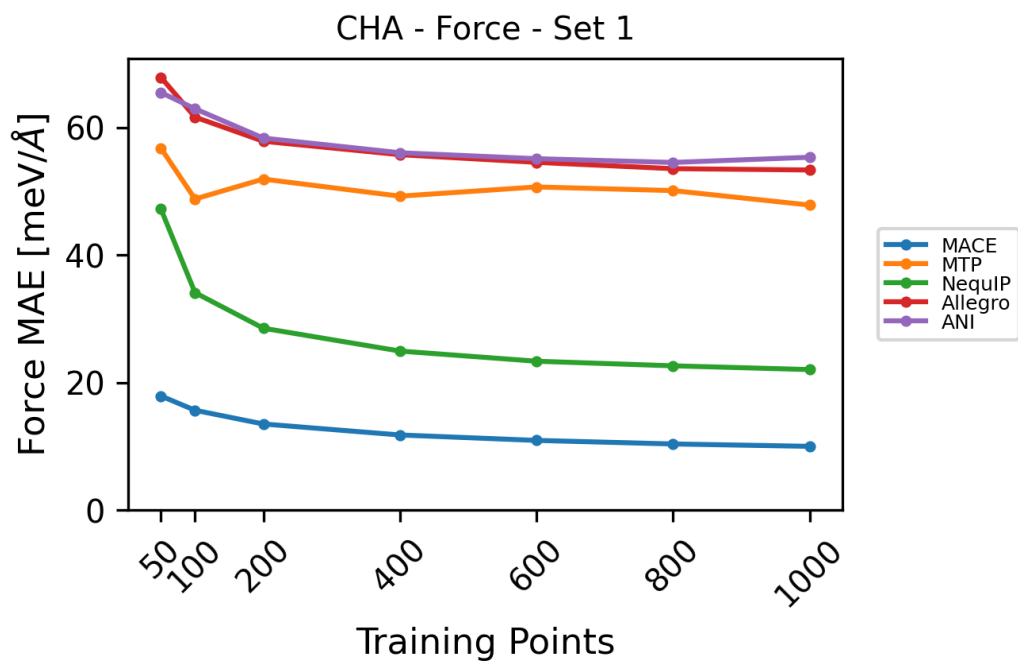
Figure S82. Energy mean absolute error vs training points for CHA, Set 1. Unit: meV/atom.
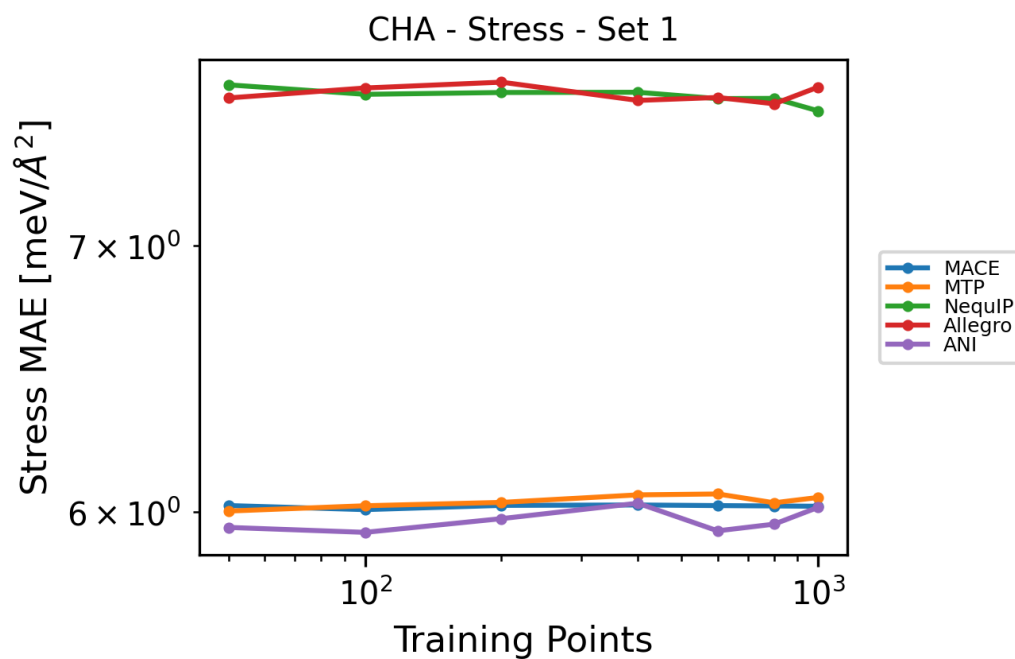
Figure S83. Force mean absolute error vs training points for CHA, Set 1. Unit: meV/Å.
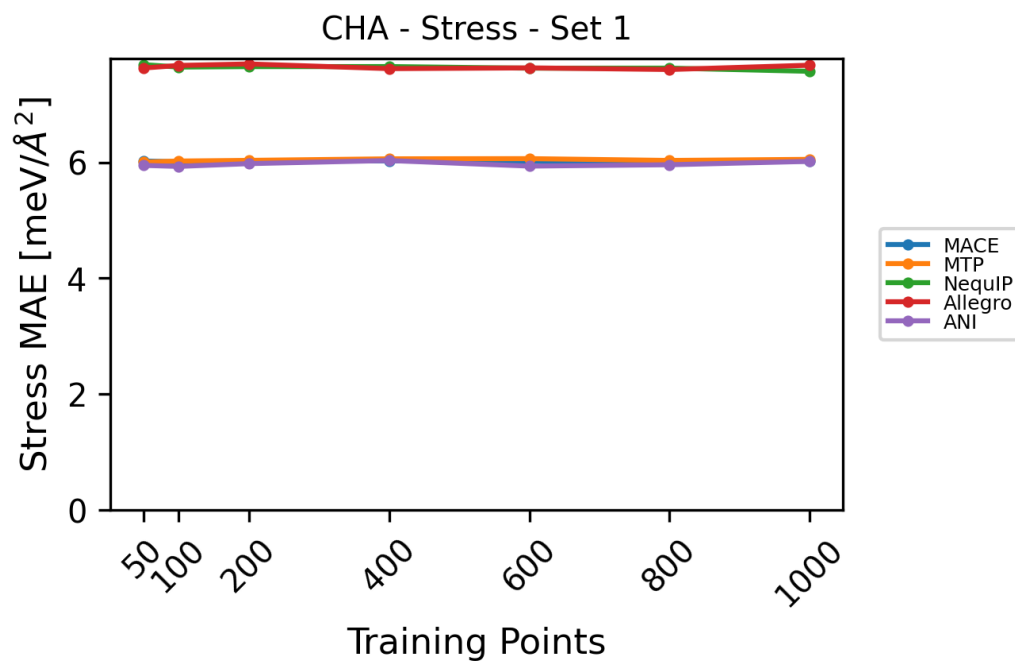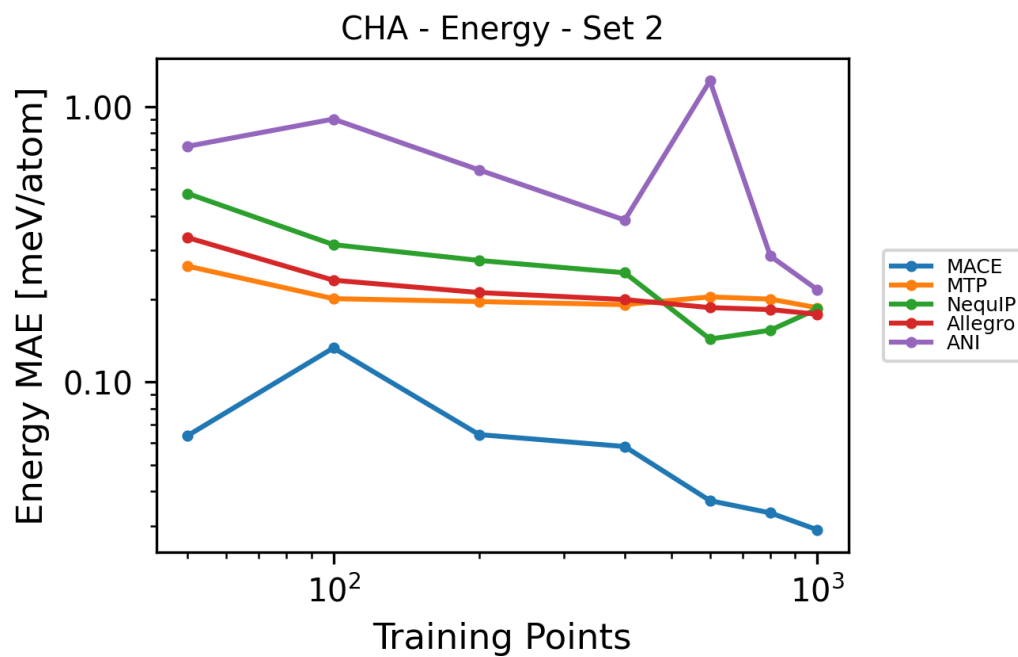
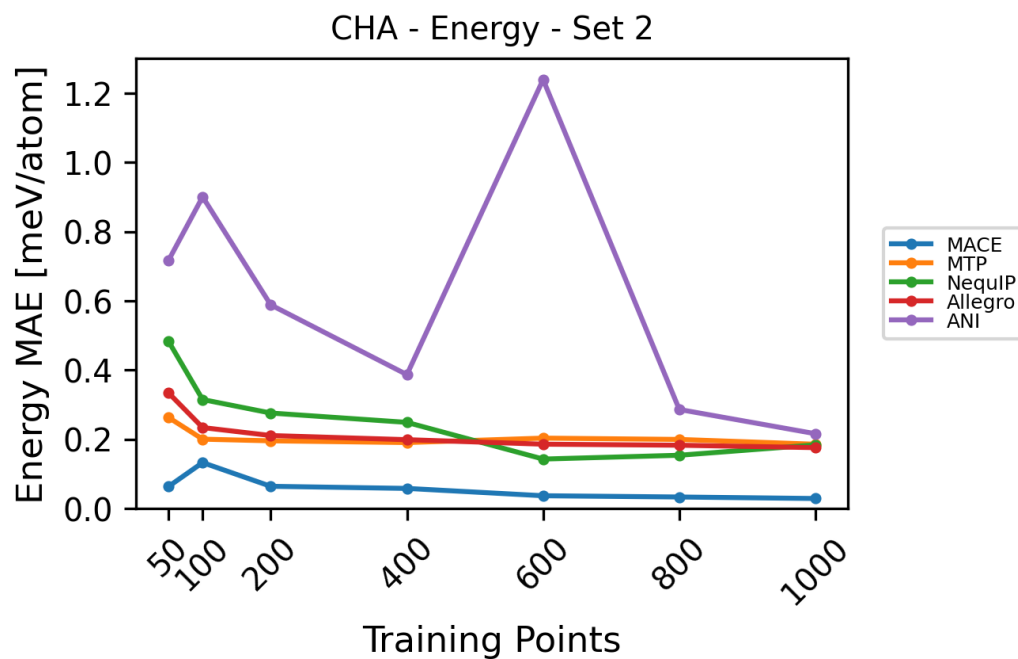**Figure S84.** Force mean absolute error vs training points for CHA, Set 1. Unit: meV/Å.

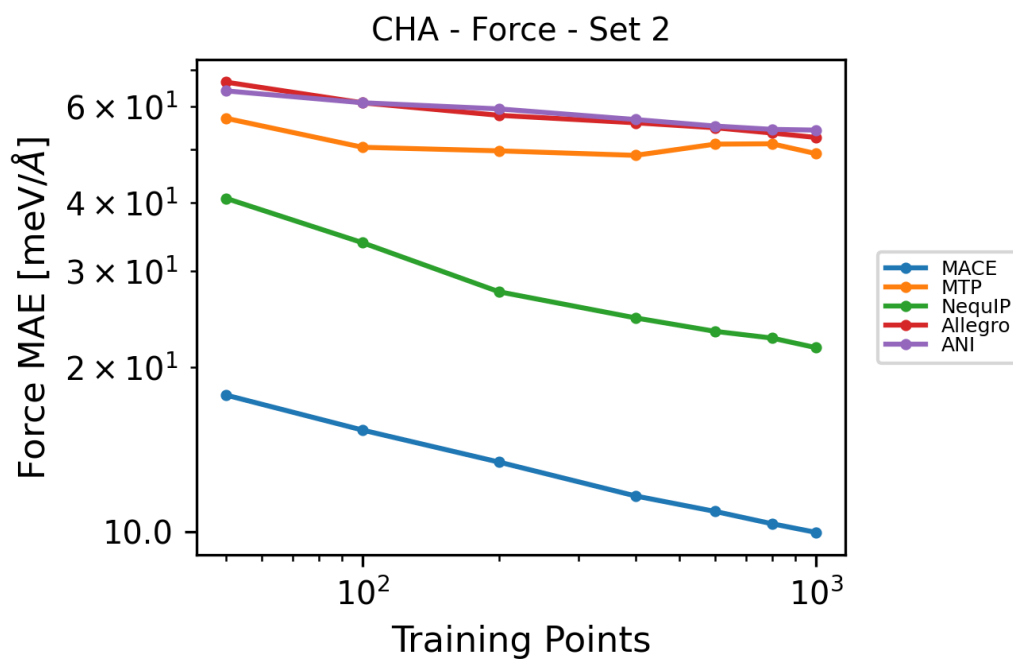**Figure S85.** Stress mean absolute error vs training points for CHA, Set 1. Unit: meV/Å².

Figure S86. Stress mean absolute error vs training points for CHA, Set 1. Unit: meV/Å².
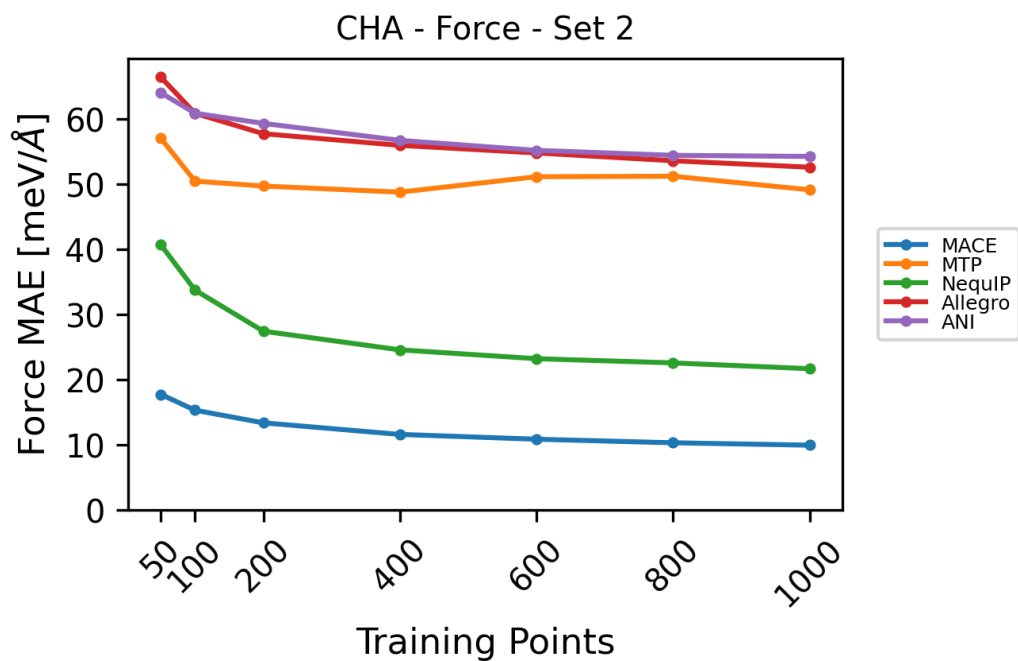
Figure S87. Energy mean absolute error vs training points for CHA, Set 2. Unit: meV/atom.
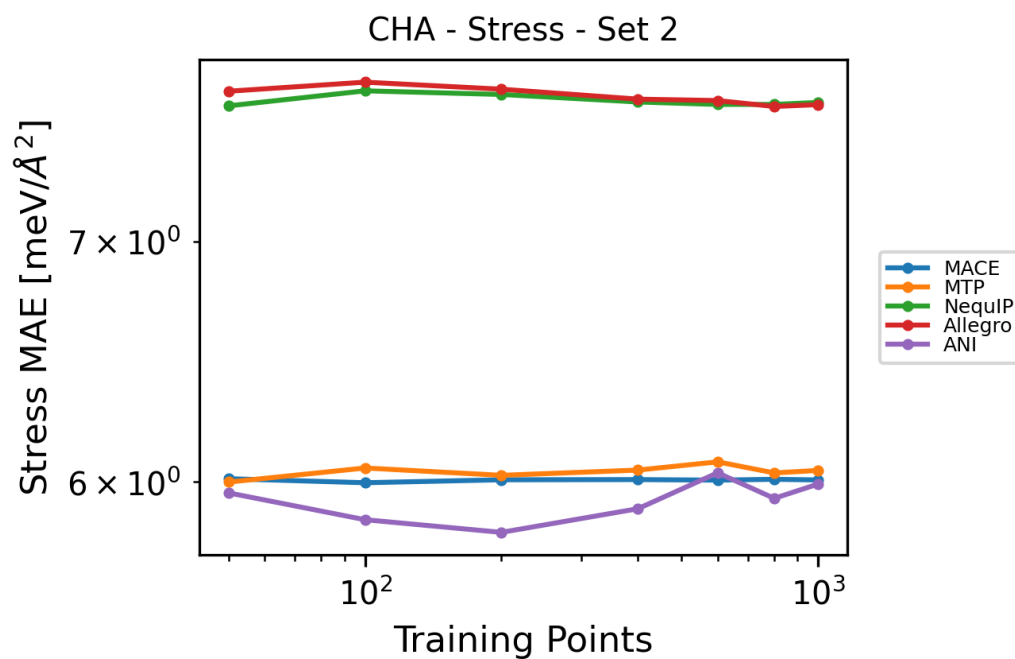
Figure S88. Energy mean absolute error vs training points for CHA, Set 2. Unit: meV/atom.

Figure S89. Force mean absolute error vs training points for CHA, Set 2. Unit: meV/Å.
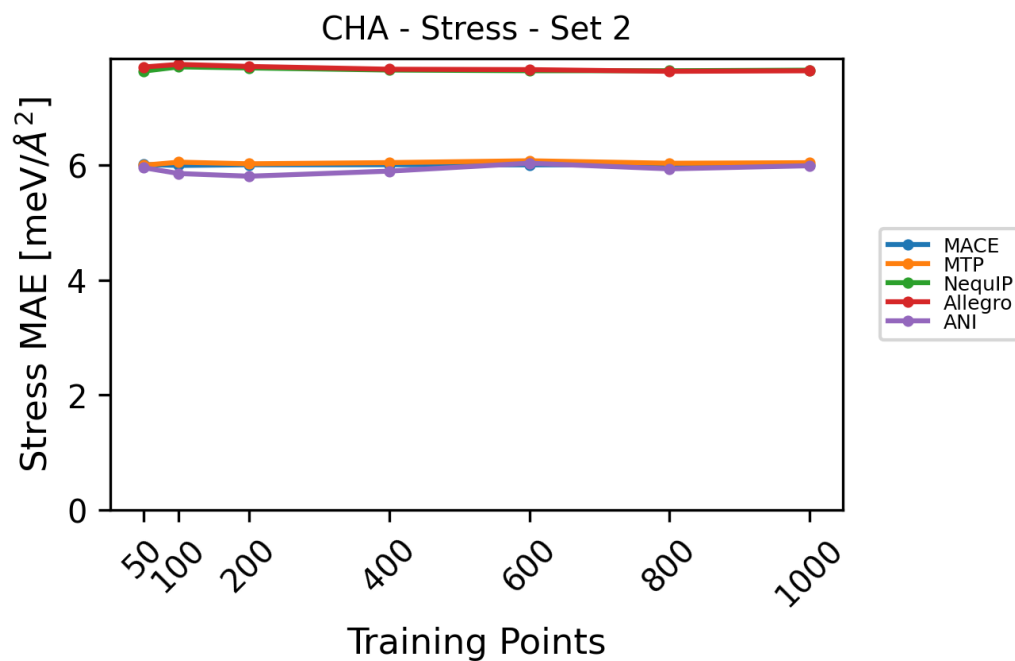
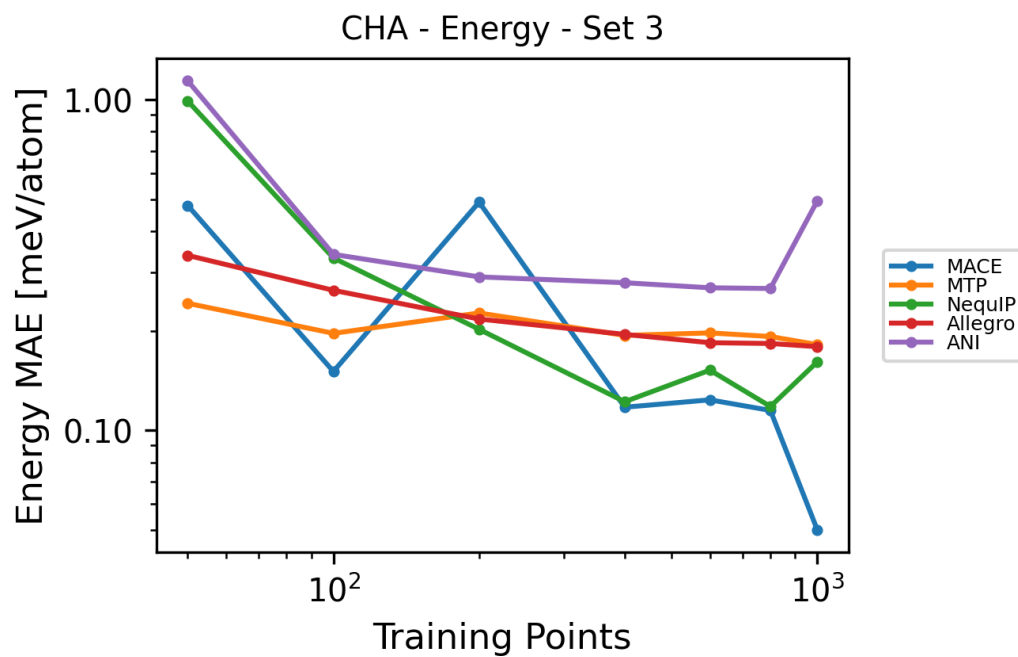**Figure S90.** Force mean absolute error vs training points for CHA, Set 2. Unit: meV/Å.

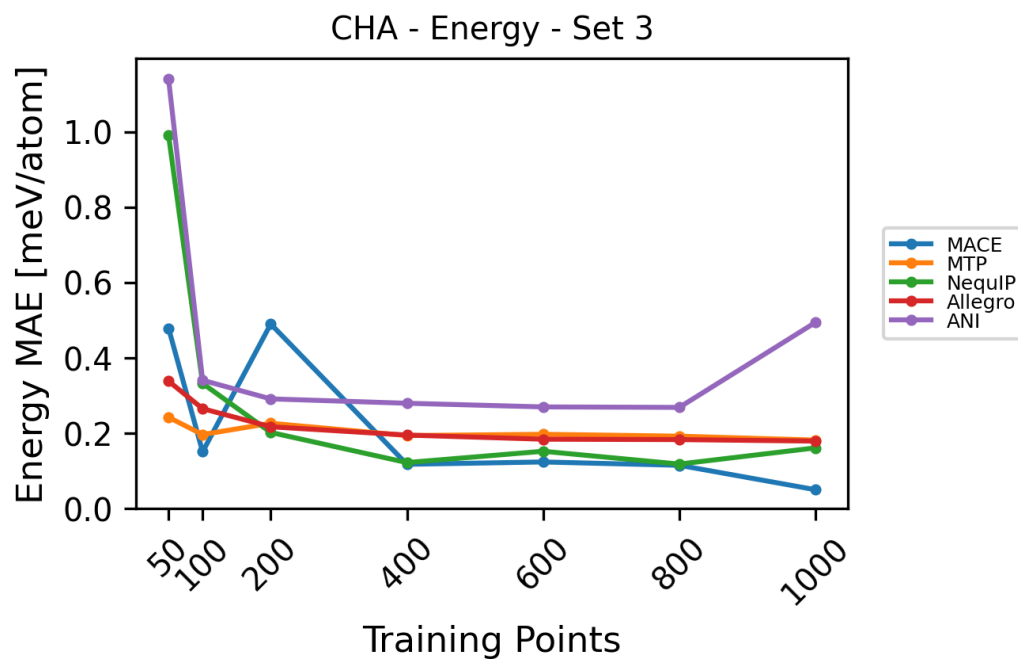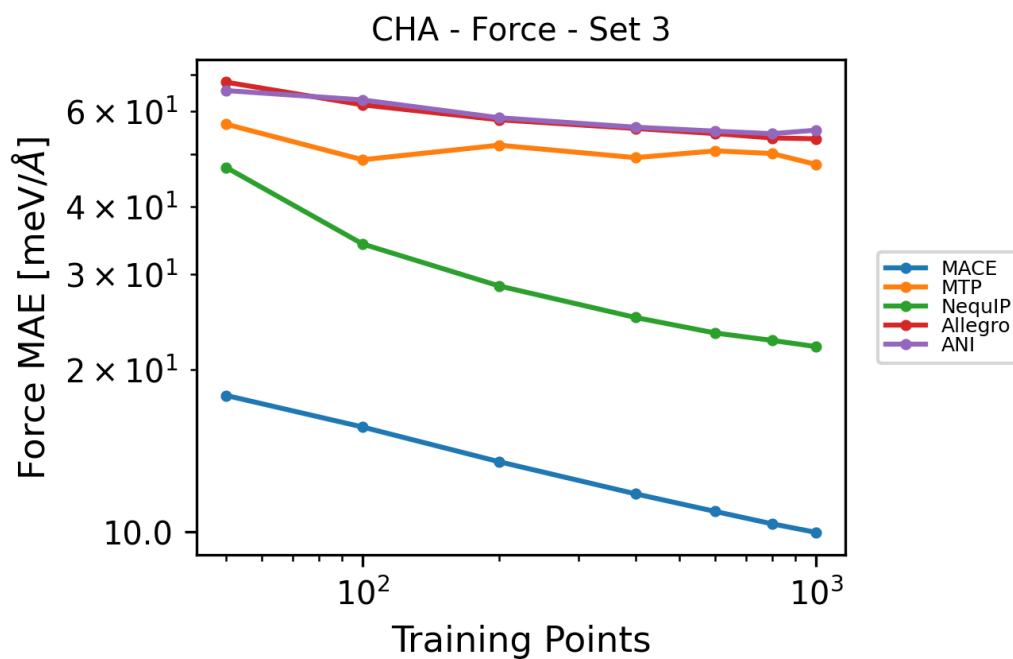**Figure S91.** Stress mean absolute error vs training points for CHA, Set 2. Unit: meV/Å².

Figure S92. Stress mean absolute error vs training points for CHA, Set 2. Unit: meV/Å².
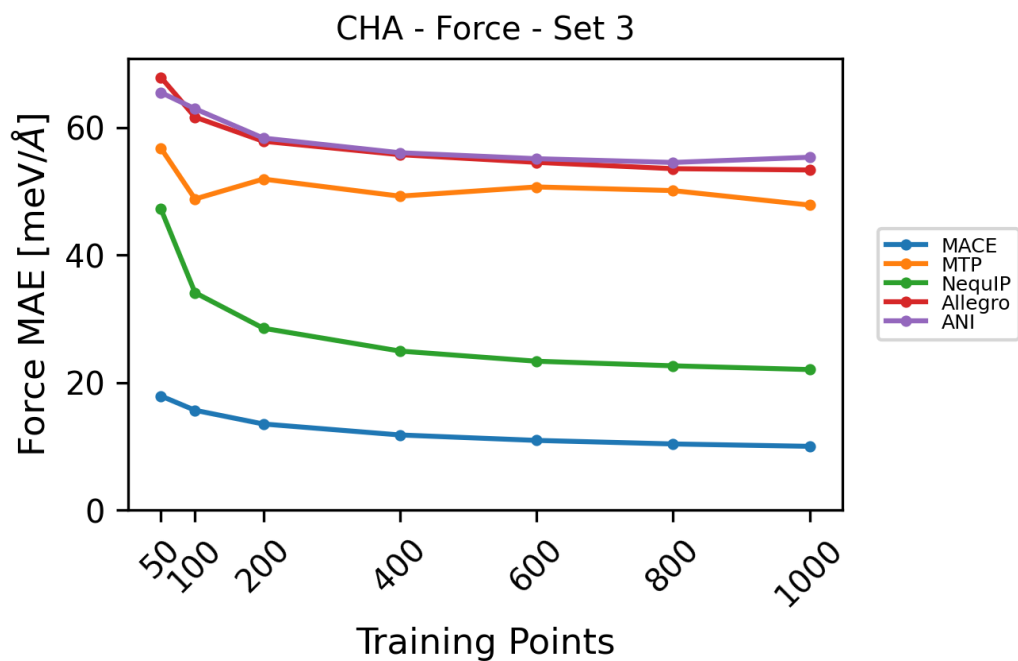
Figure S93. Energy mean absolute error vs training points for CHA, Set 3. Unit: meV/atom.
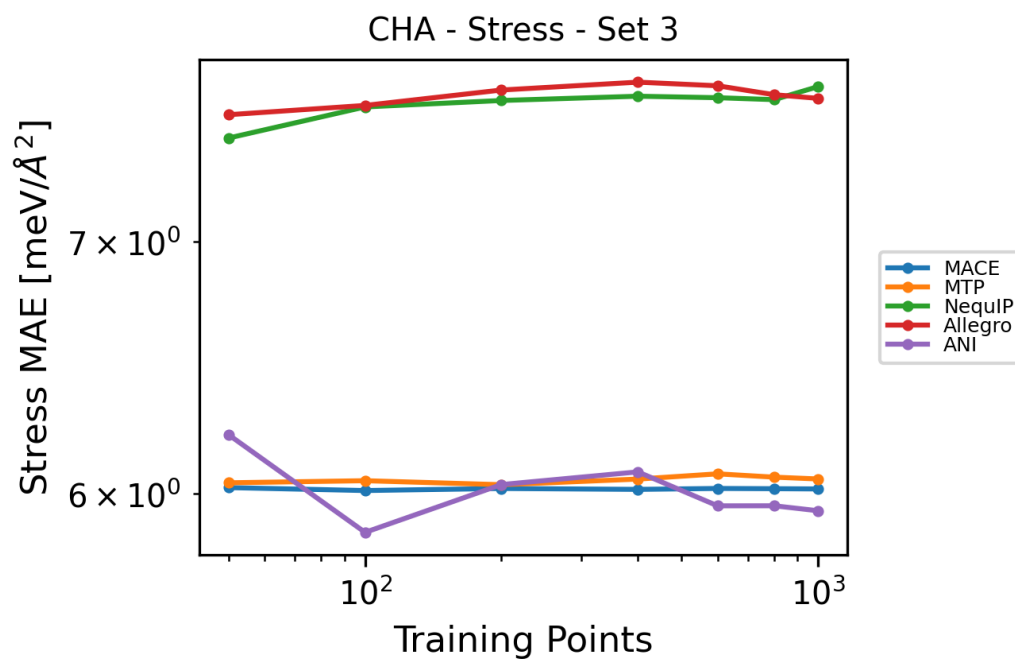
Figure S94. Energy mean absolute error vs training points for CHA, Set 3. Unit: meV/atom.
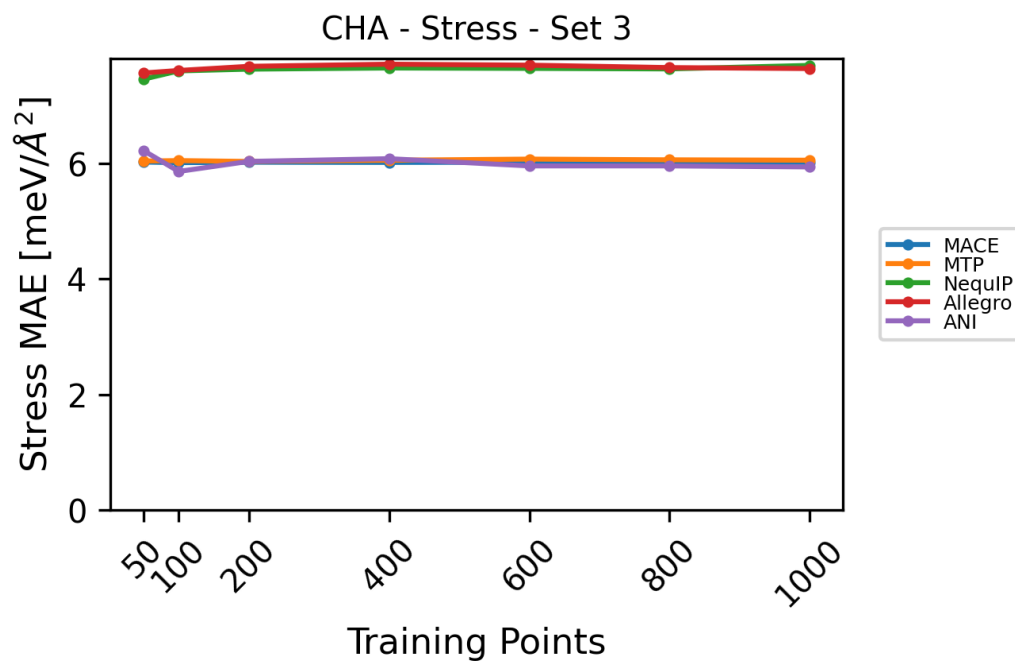
Figure S95. Force mean absolute error vs training points for CHA, Set 3. Unit: meV/Å.
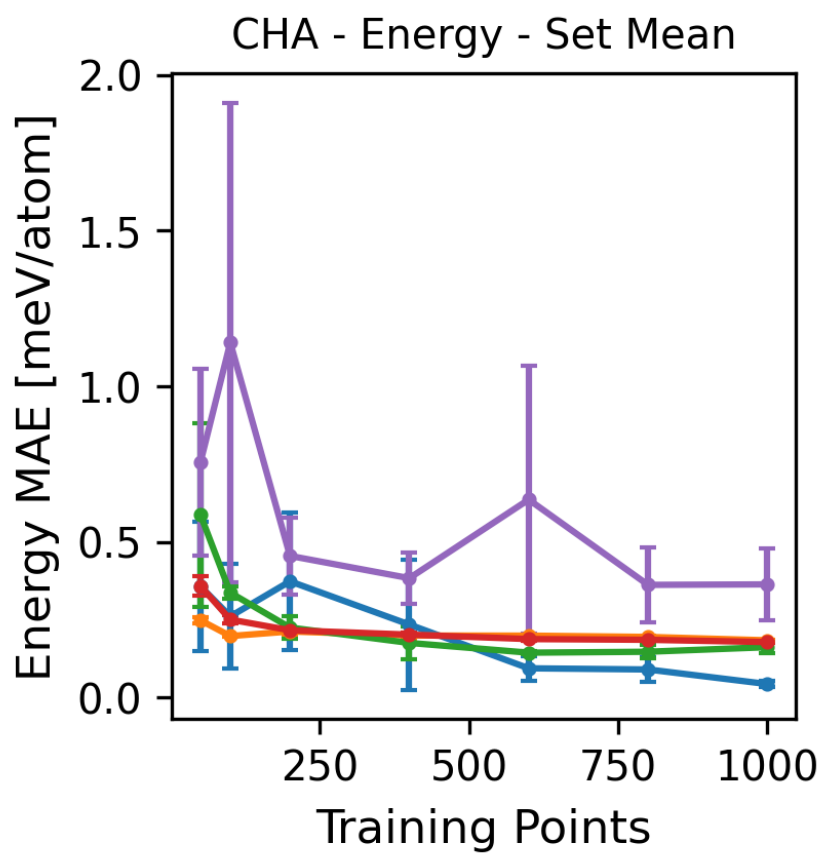
Figure S96. Force mean absolute error vs training points for CHA, Set 3. Unit: meV/Å.

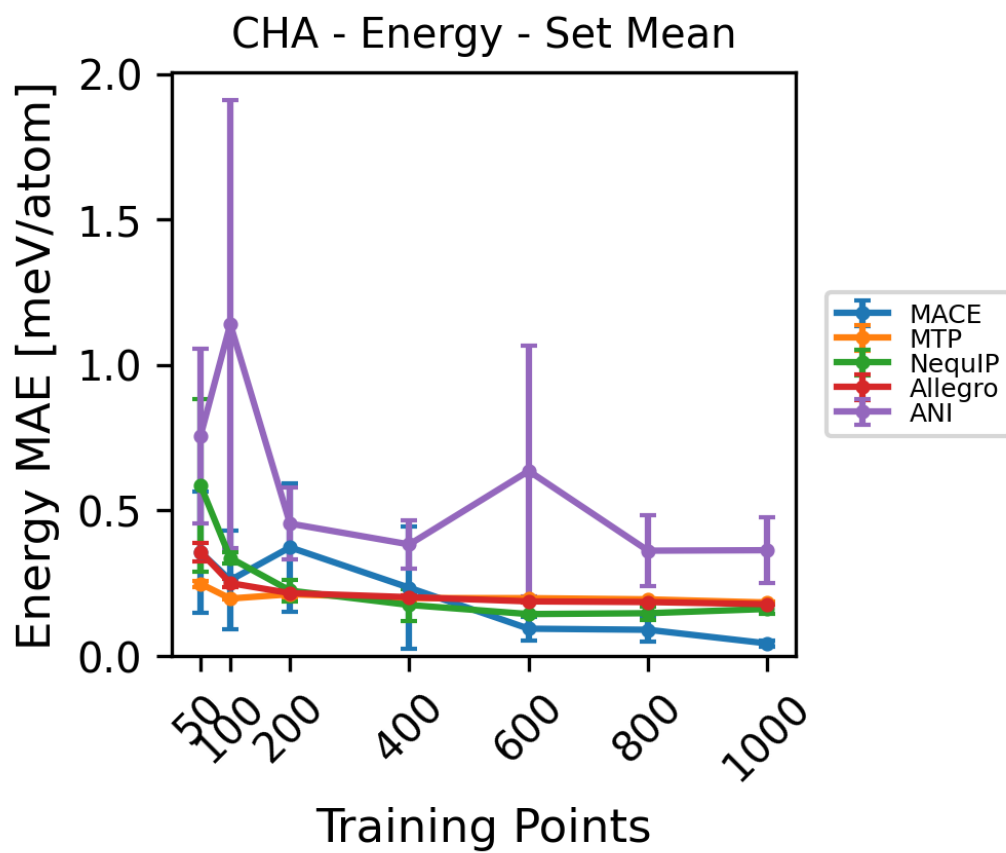**Figure S97.** Stress mean absolute error vs training points for CHA, Set 3. Unit: meV/Å².

Figure S98. Stress mean absolute error vs training points for CHA, Set 3. Unit: meV/Å².
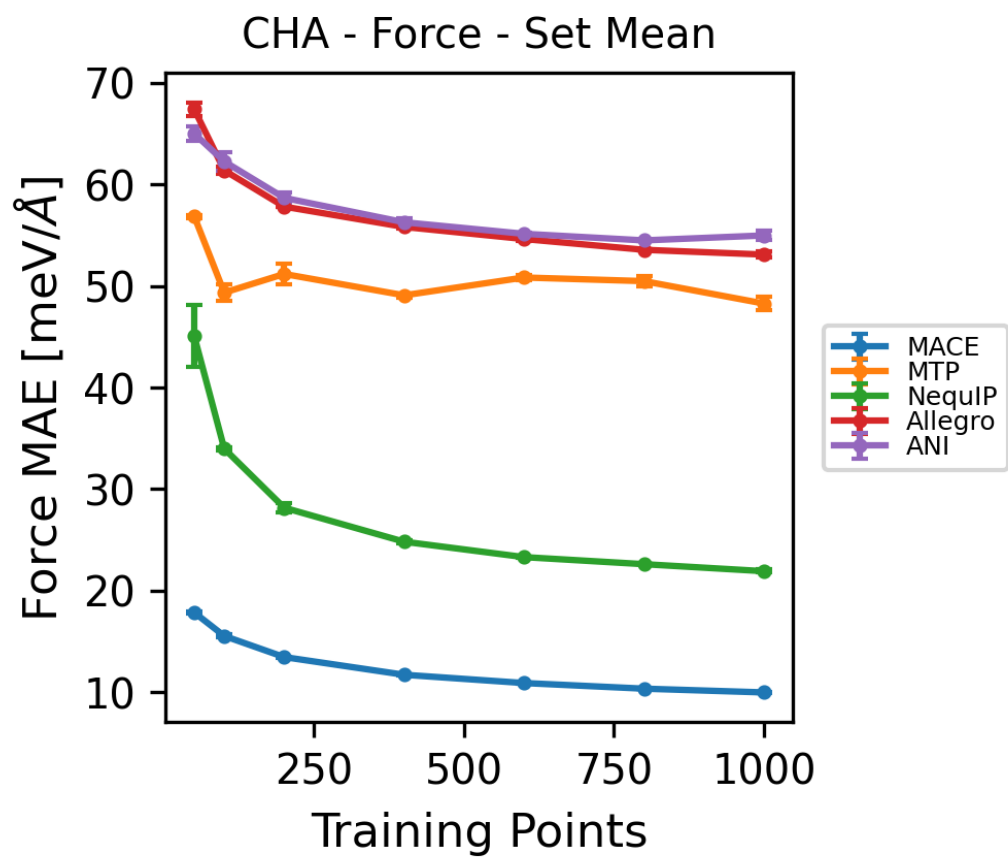
Figure S99. Energy mean absolute error vs training points for CHA, Set mean. Unit: meV/atom.
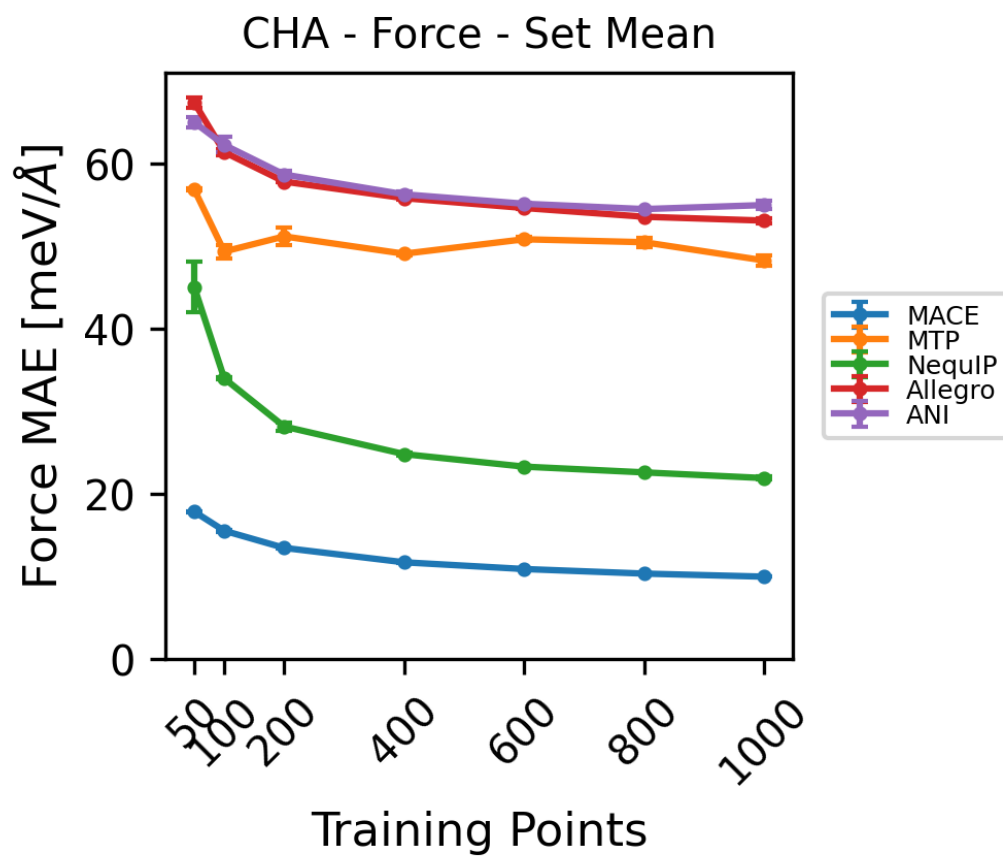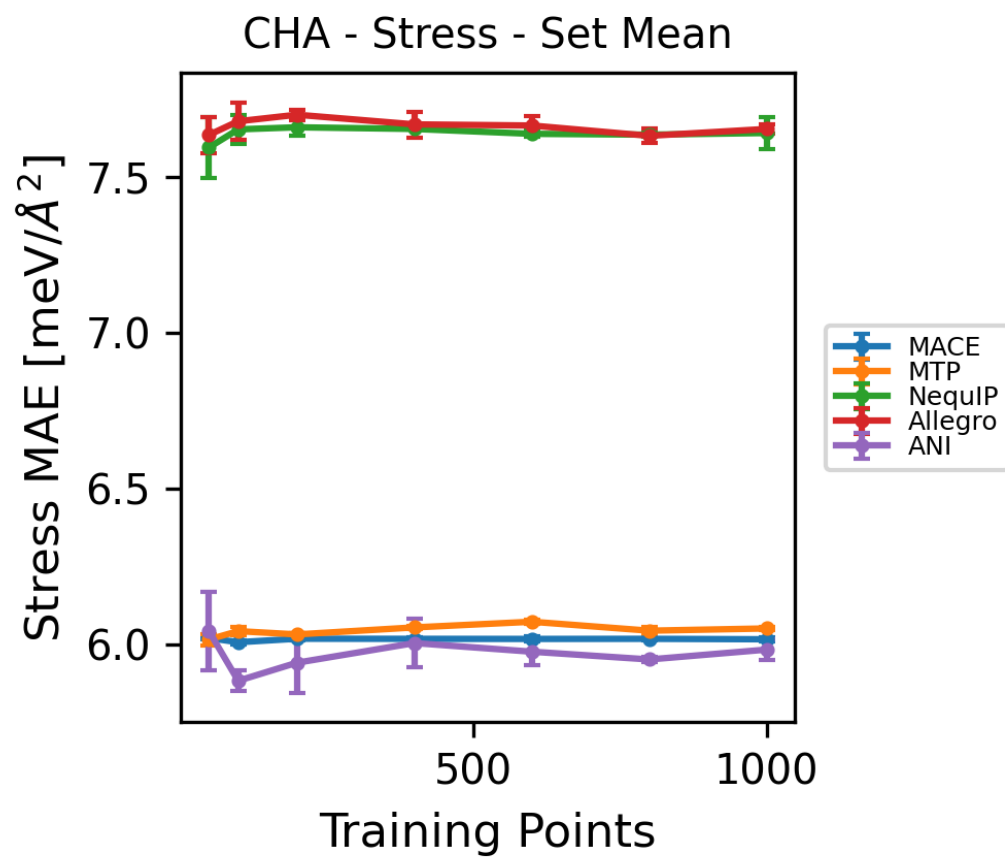
Figure S100. Energy mean absolute error vs training points for CHA, Set mean. Unit: meV/atom.
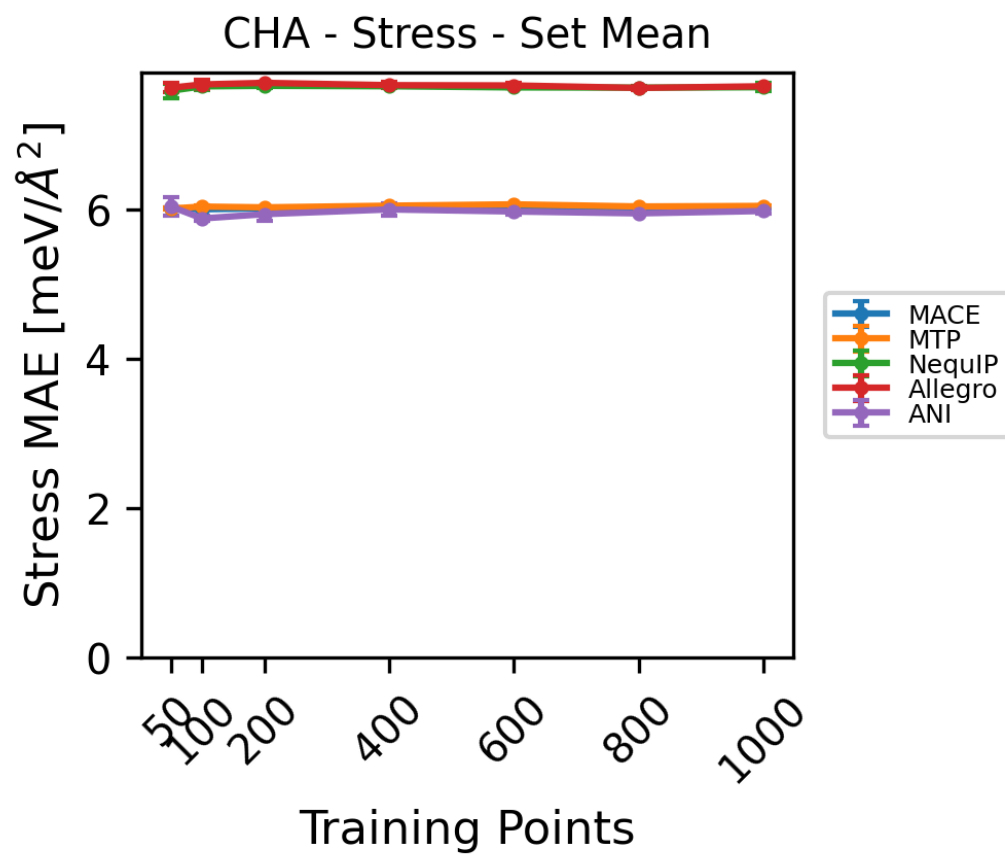
Figure S101. Force mean absolute error vs training points for CHA, Set mean. Unit: meV/Å.

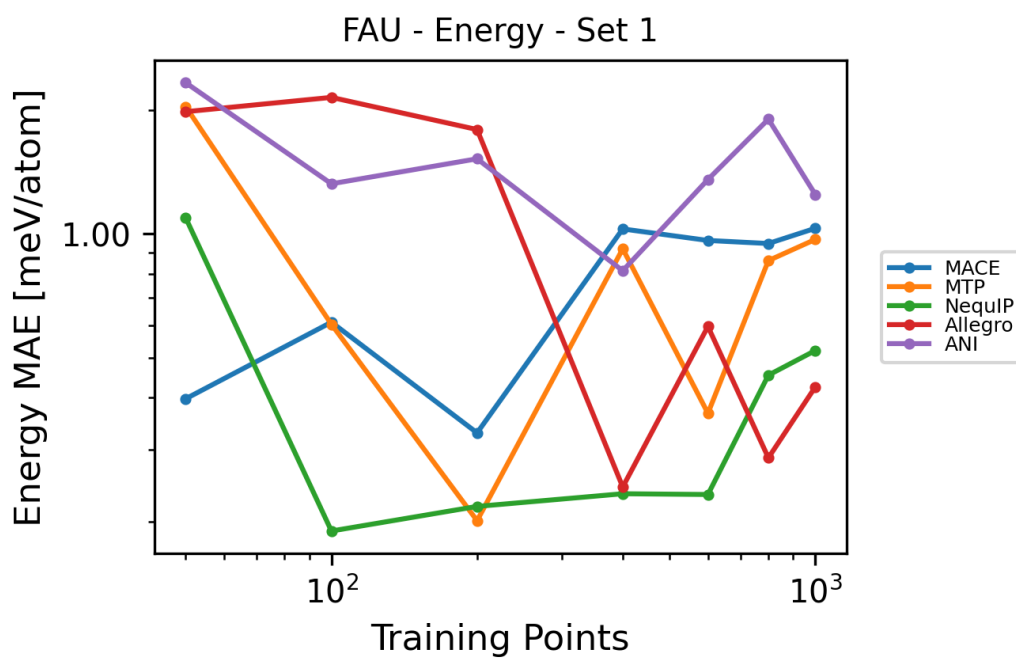**Figure S102.** Force mean absolute error vs training points for CHA, Set mean. Unit: meV/Å.

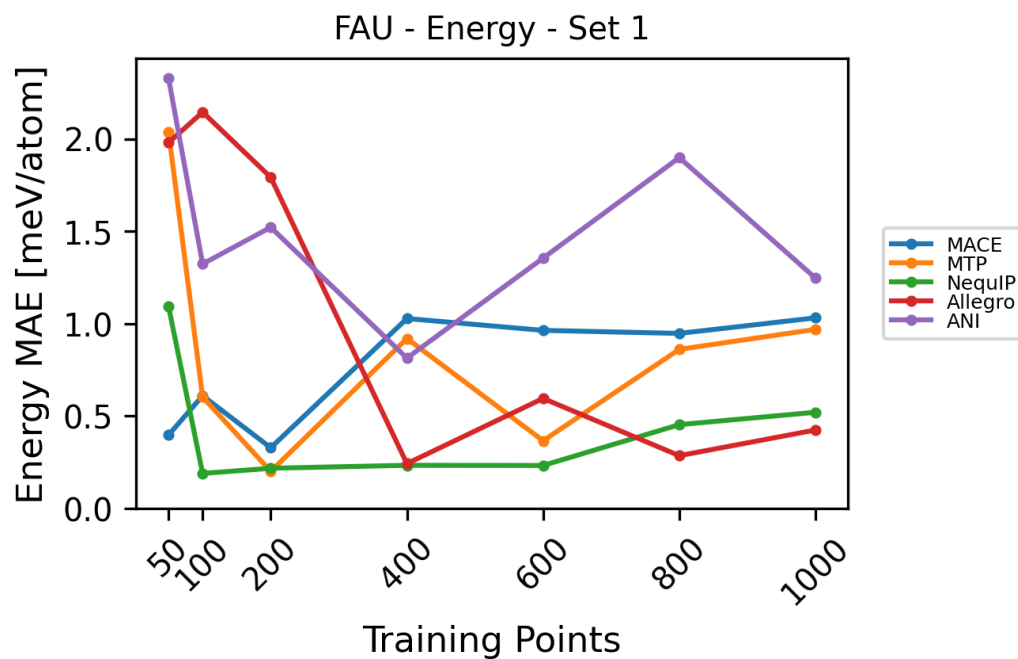**Figure S103.** Stress mean absolute error vs training points for CHA, Set mean. Unit: meV/Å².

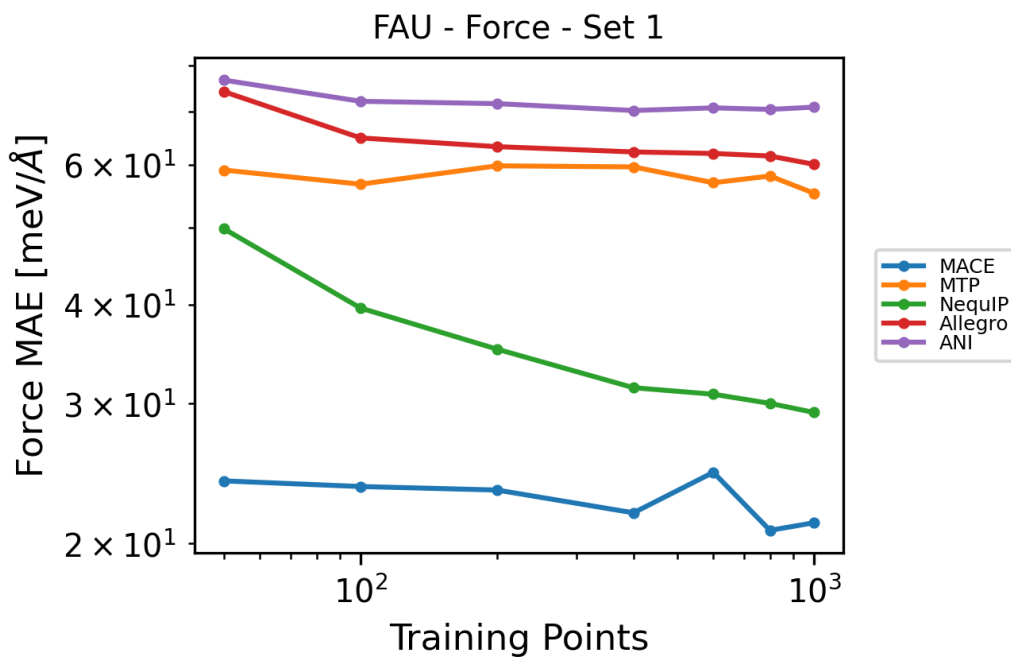**Figure S104.** Stress mean absolute error vs training points for CHA, Set mean. Unit: meV/Å².

FAU

Figure S105. Energy mean absolute error vs training points for FAU, Set 1. Unit: meV/atom.
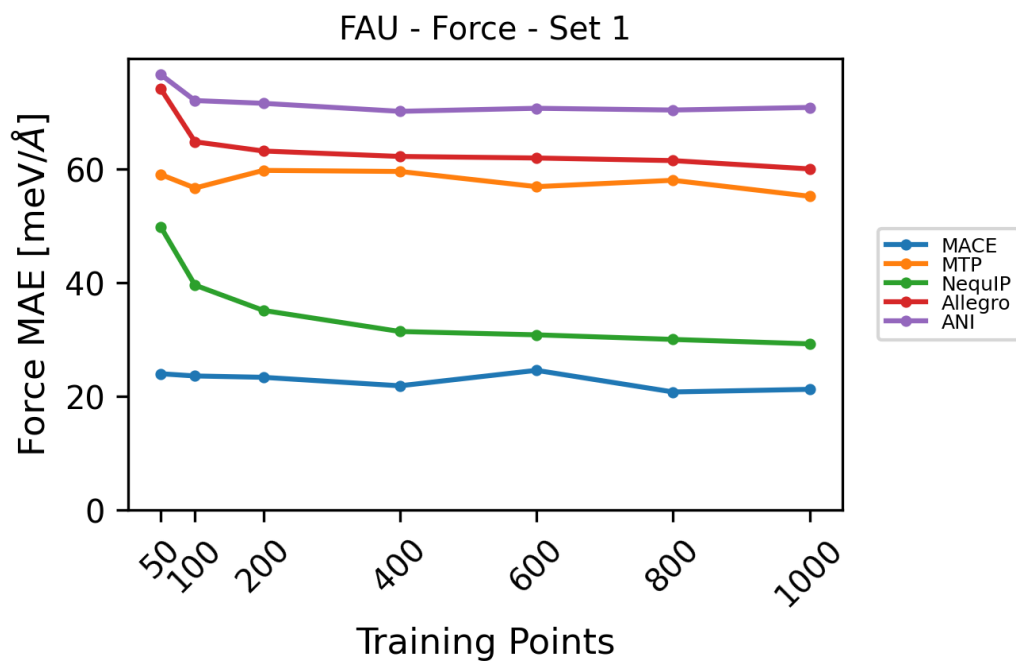
Figure S106. Energy mean absolute error vs training points for FAU, Set 1. Unit: meV/atom.
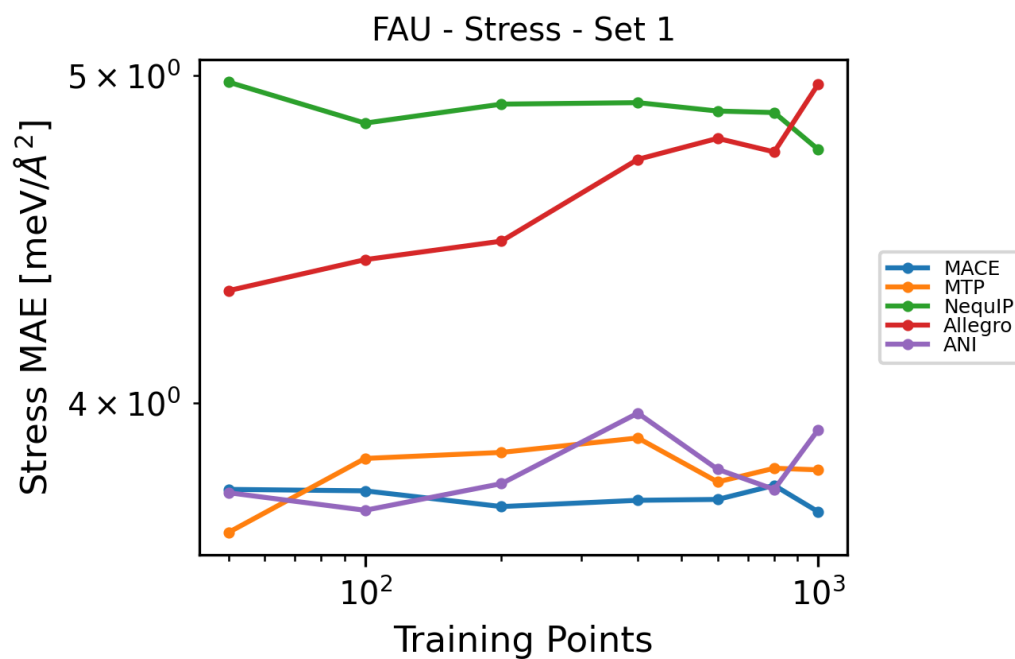
Figure S107. Force mean absolute error vs training points for FAU, Set 1. Unit: meV/Å.
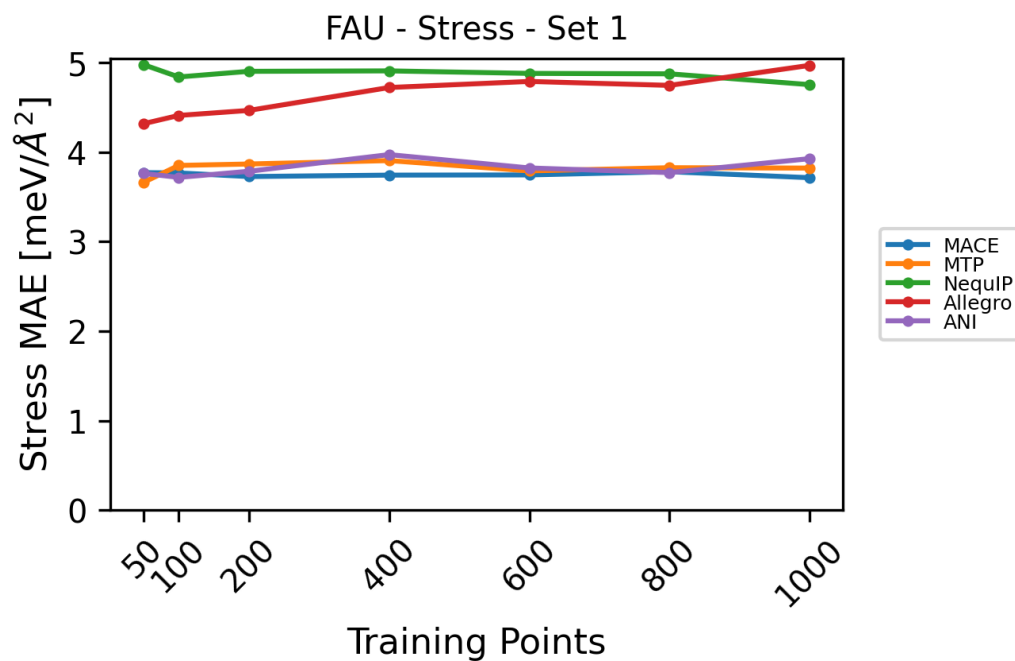
Figure S108. Force mean absolute error vs training points for FAU, Set 1. Unit: meV/Å.

Figure S109. Stress mean absolute error vs training points for FAU, Set 1. Unit: meV/Å².

Figure S110. Stress mean absolute error vs training points for FAU, Set 1. Unit: meV/Å².

Figure S111. Energy mean absolute error vs training points for FAU, Set 2. Unit: meV/atom.

Figure S112. Energy mean absolute error vs training points for FAU, Set 2. Unit: meV/atom.

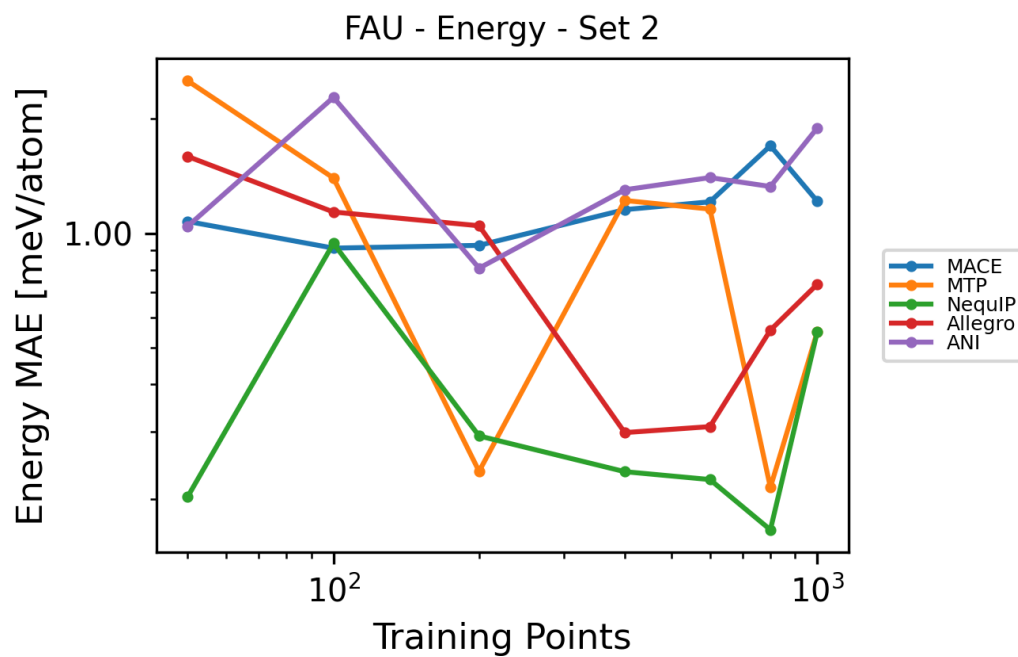**Figure S113.** Force mean absolute error vs training points for FAU, Set 2. Unit: meV/Å.

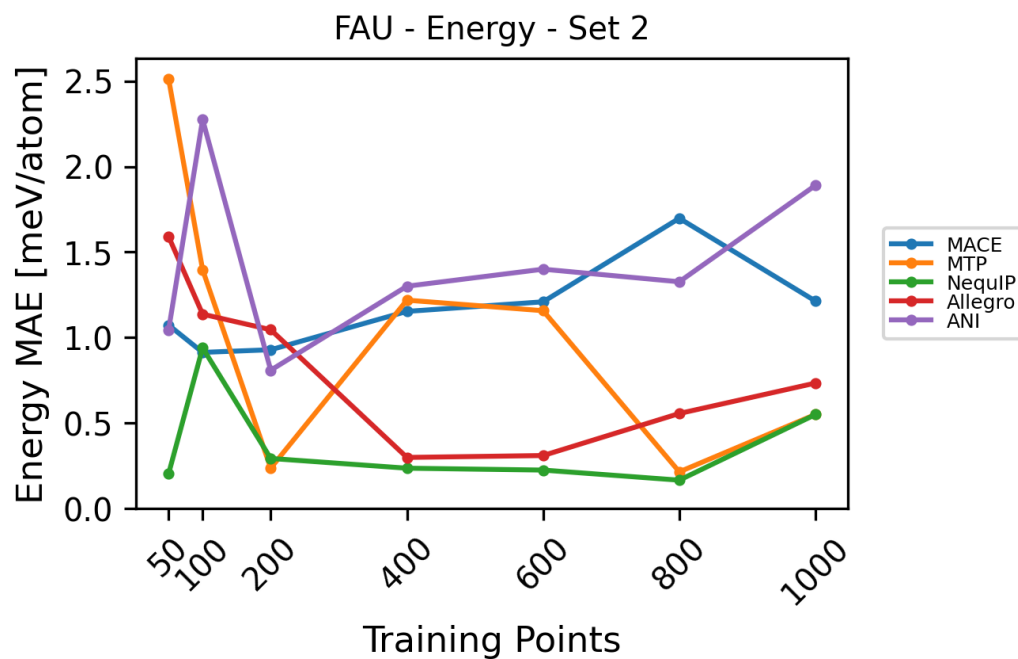**Figure S114.** Force mean absolute error vs training points for FAU, Set 2. Unit: meV/Å.

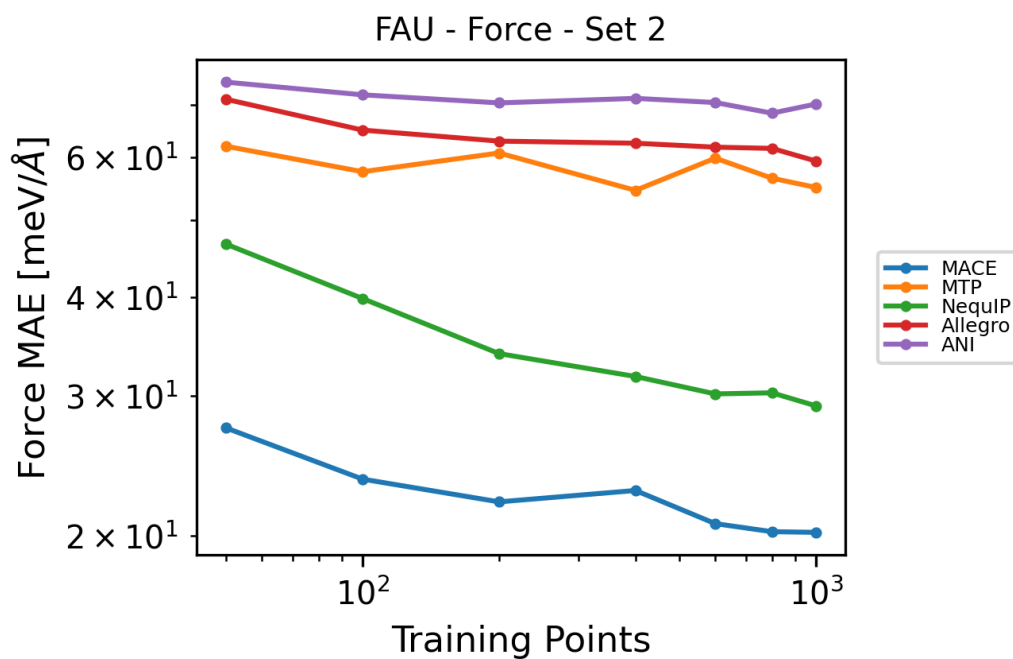**Figure S115.** Stress mean absolute error vs training points for FAU, Set 2. Unit: meV/Å².

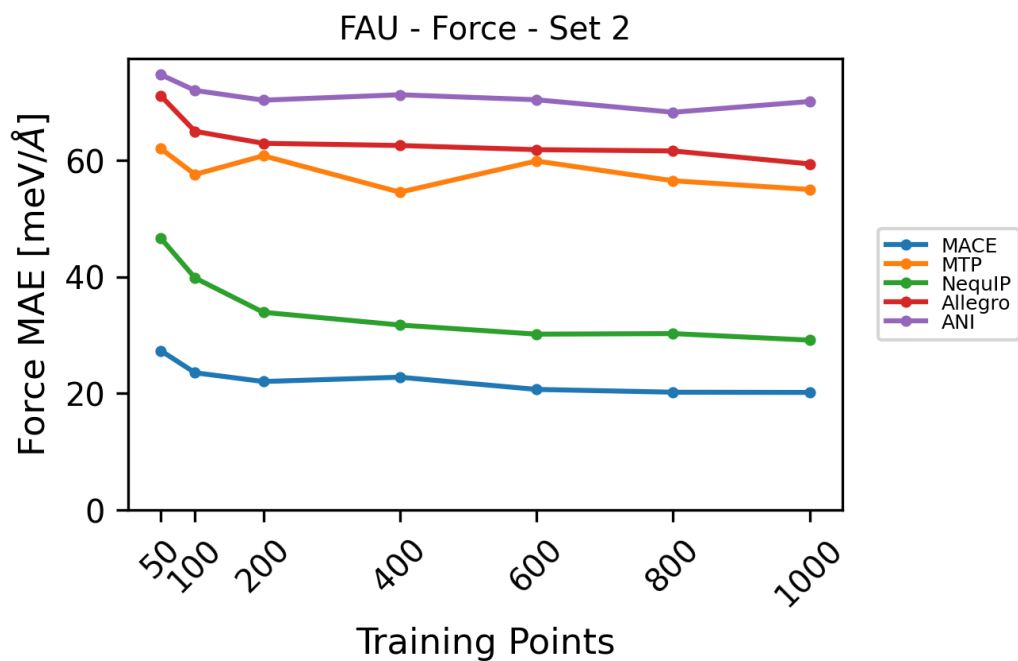**Figure S116.** Stress mean absolute error vs training points for FAU, Set 2. Unit: meV/Å².

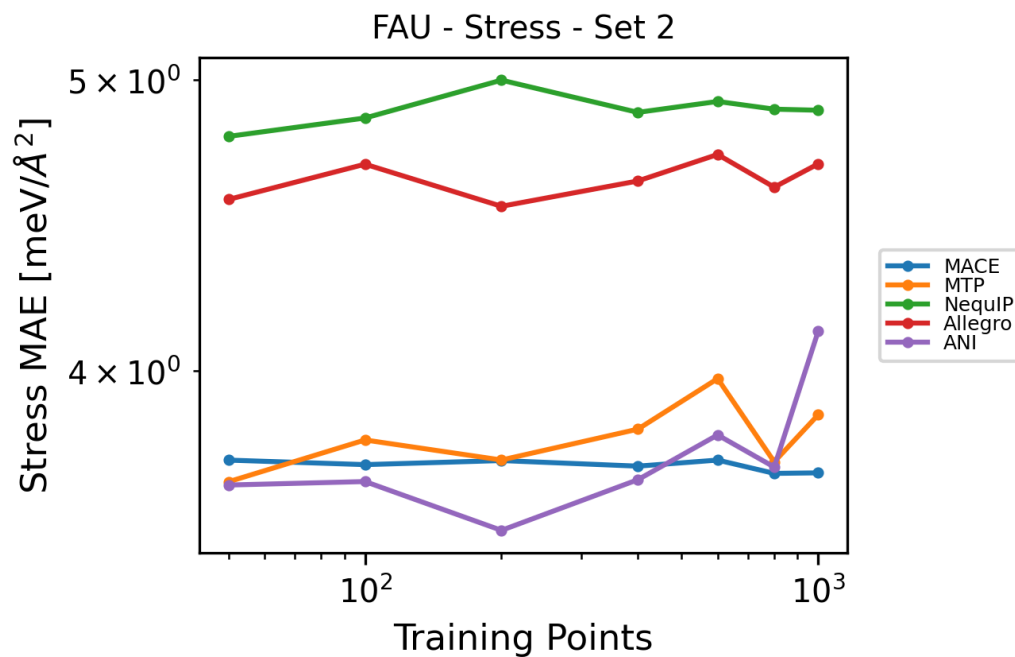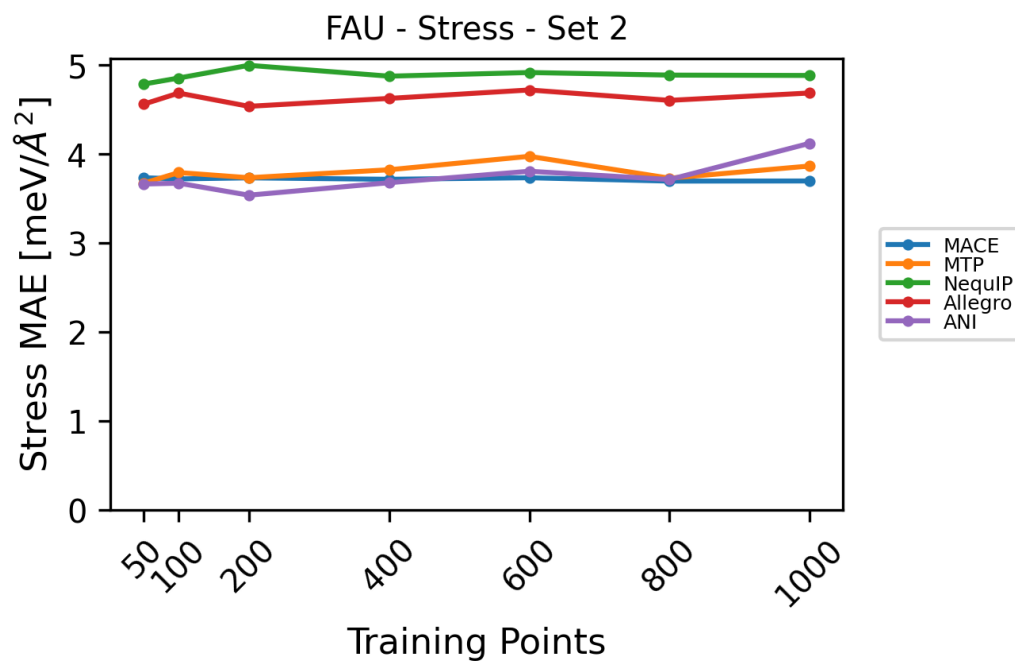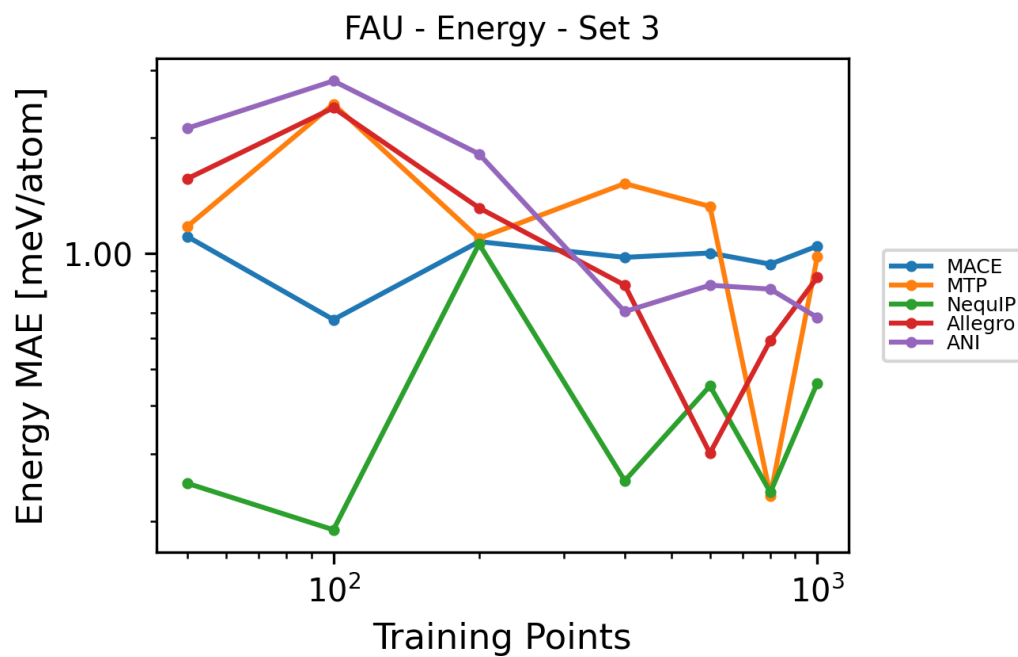**Figure S117.** Energy mean absolute error vs training points for FAU, Set 3. Unit: meV/atom.

Figure S118. Energy mean absolute error vs training points for FAU, Set 3. Unit: meV/atom.

Figure S119. Force mean absolute error vs training points for FAU, Set 3. Unit: meV/Å.

Figure S120. Force mean absolute error vs training points for FAU, Set 3. Unit: meV/Å.

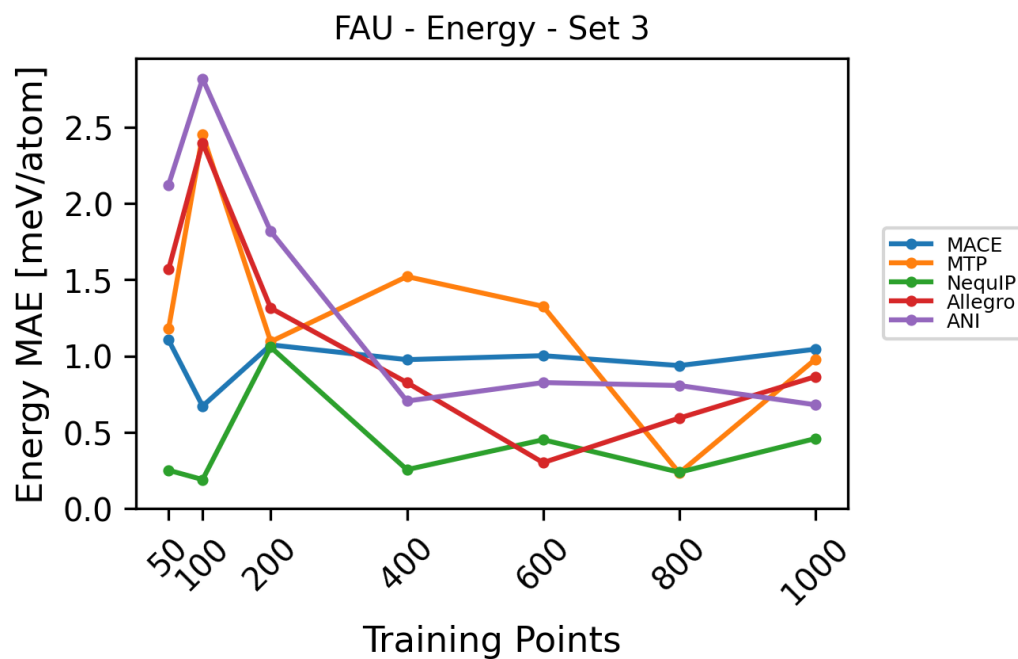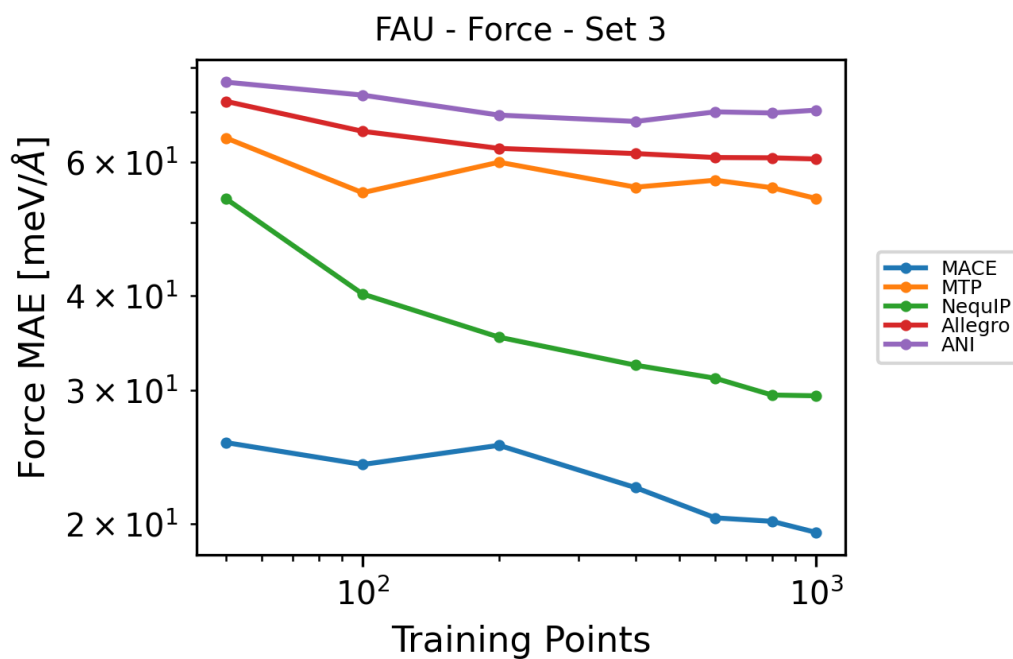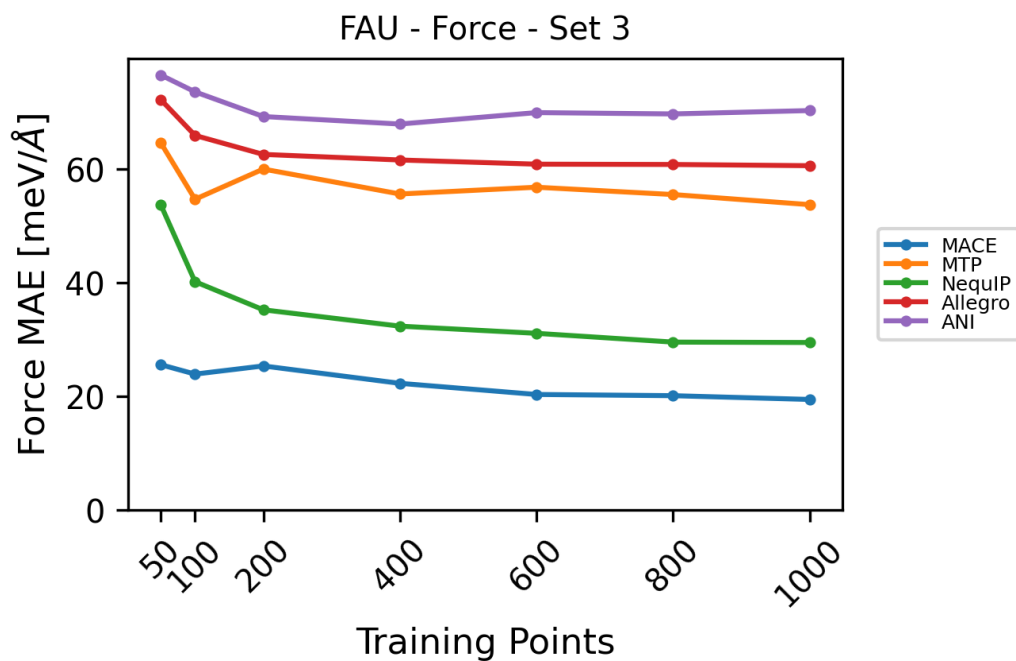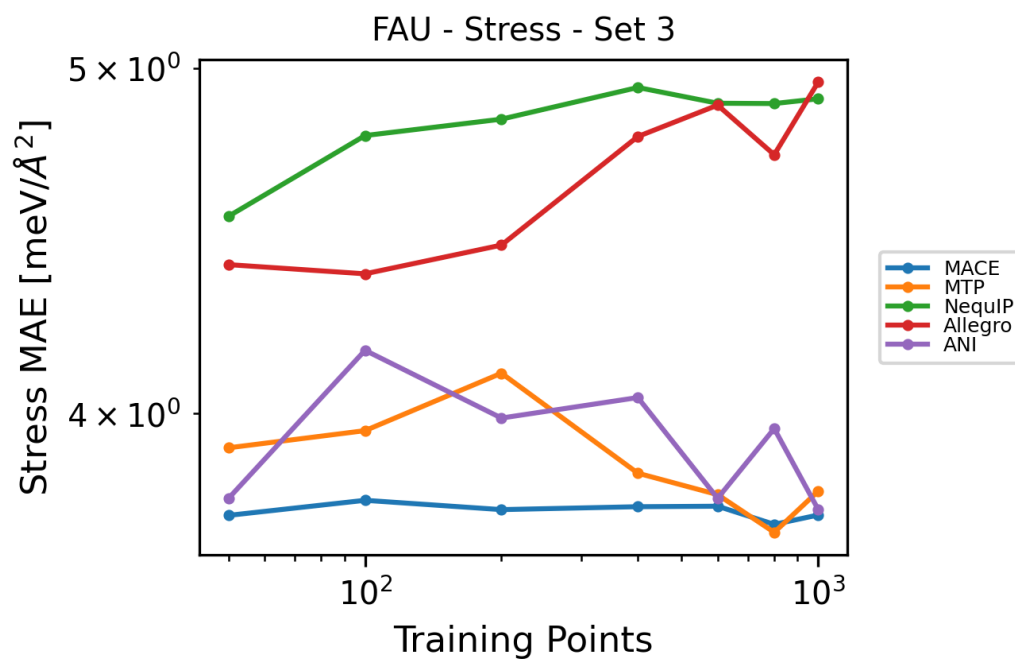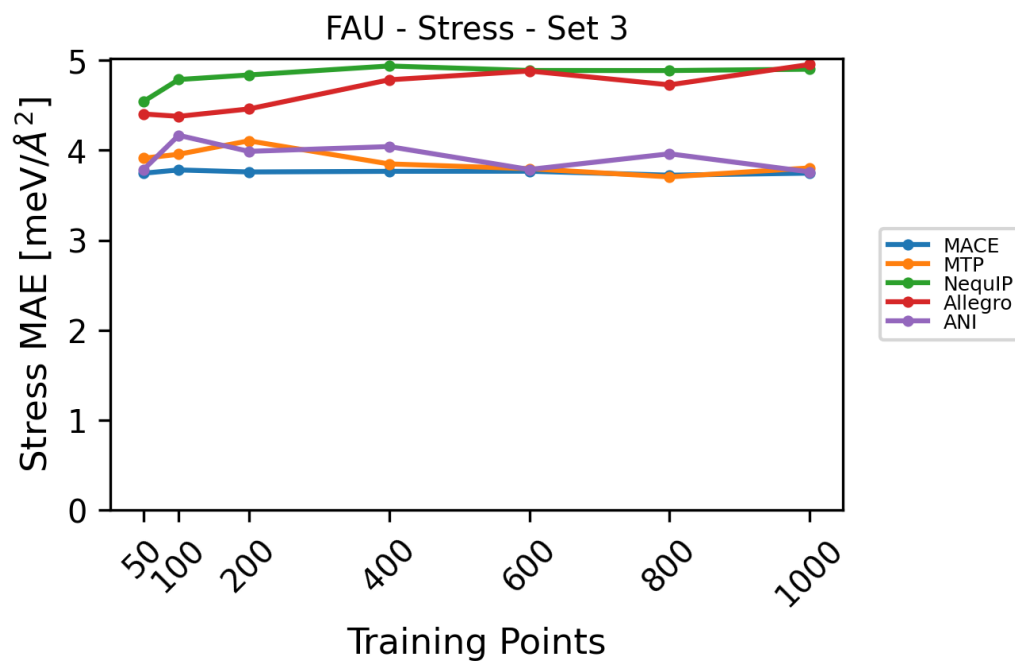**Figure S121.** Stress mean absolute error vs training points for FAU, Set 3. Unit: meV/Å².

Figure S122. Stress mean absolute error vs training points for FAU, Set 3. Unit: meV/Å².

Figure S123. Energy mean absolute error vs training points for FAU, Set mean. Unit: meV/atom.

Figure S124. Energy mean absolute error vs training points for FAU, Set mean. Unit: meV/atom.

Figure S125. Force mean absolute error vs training points for FAU, Set mean. Unit: meV/Å.
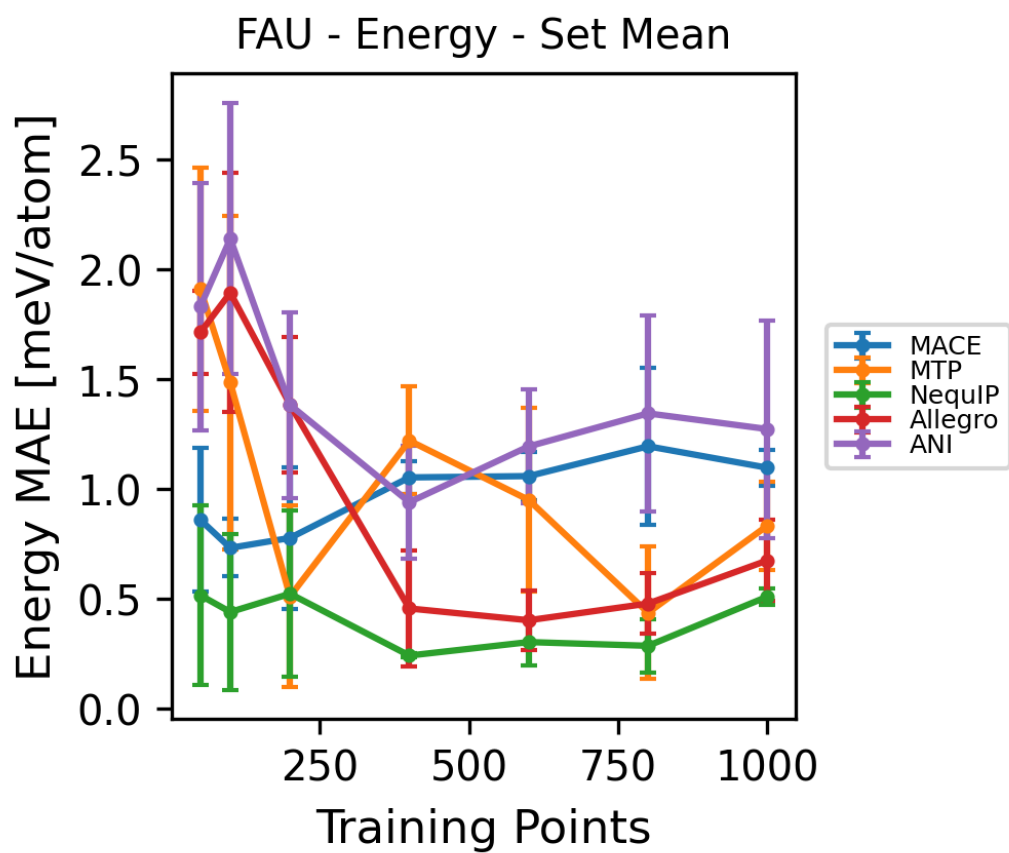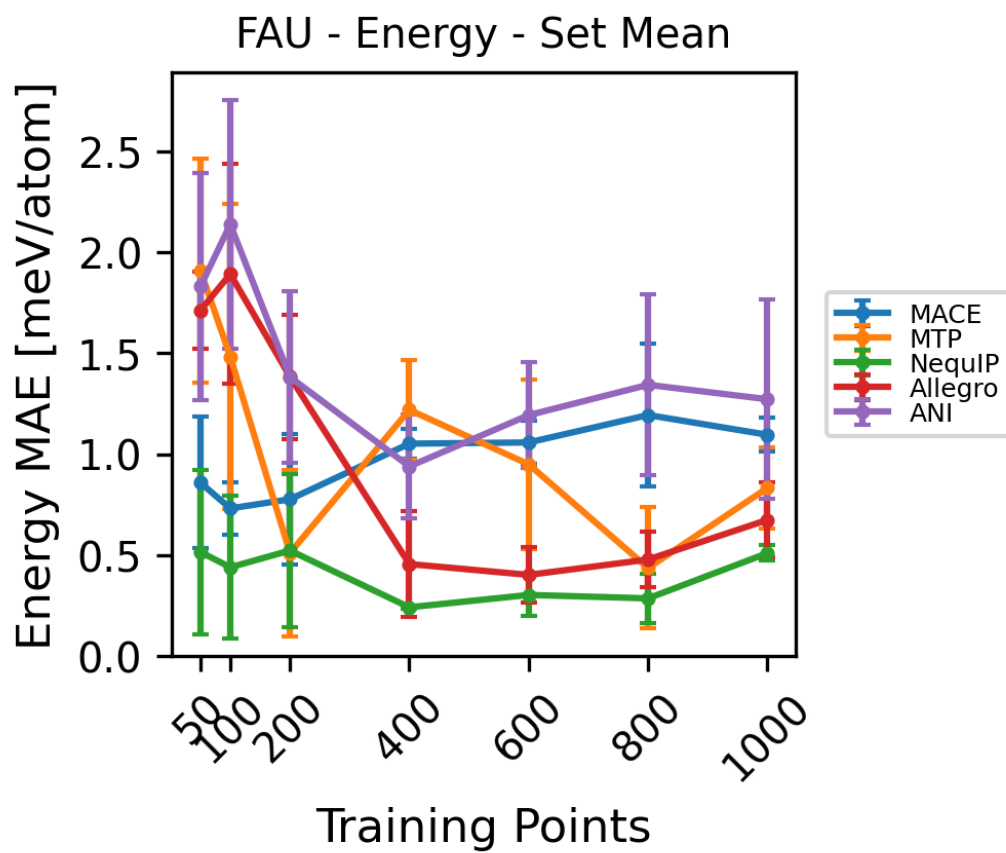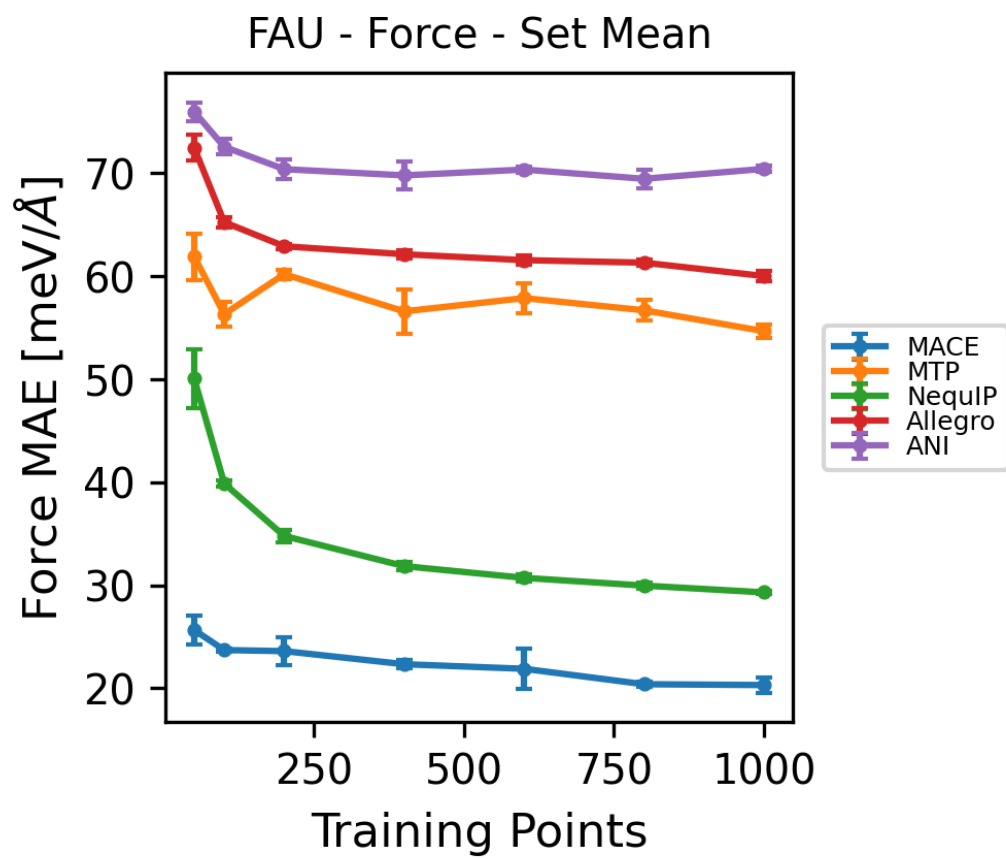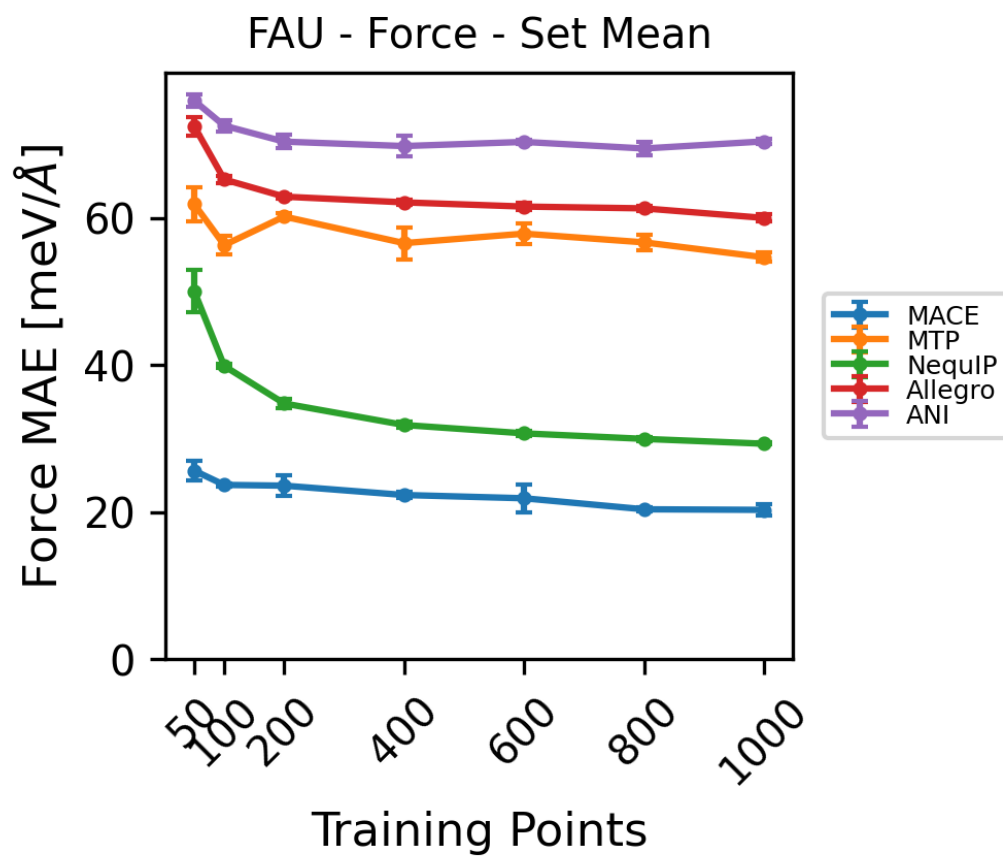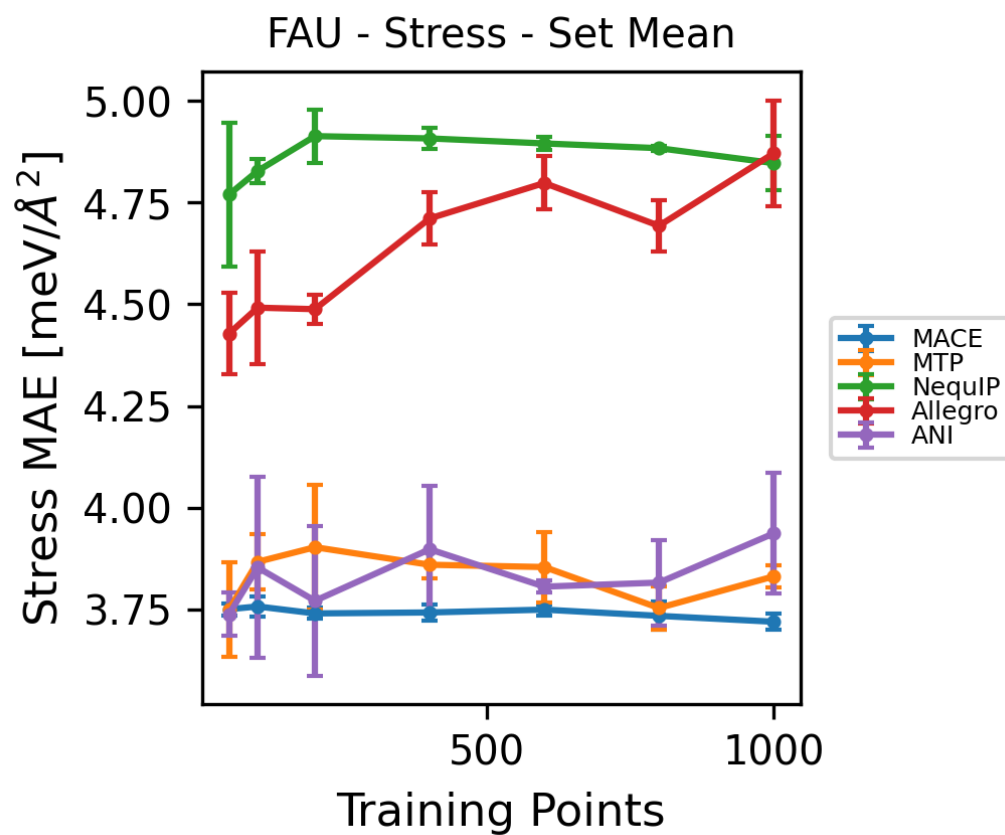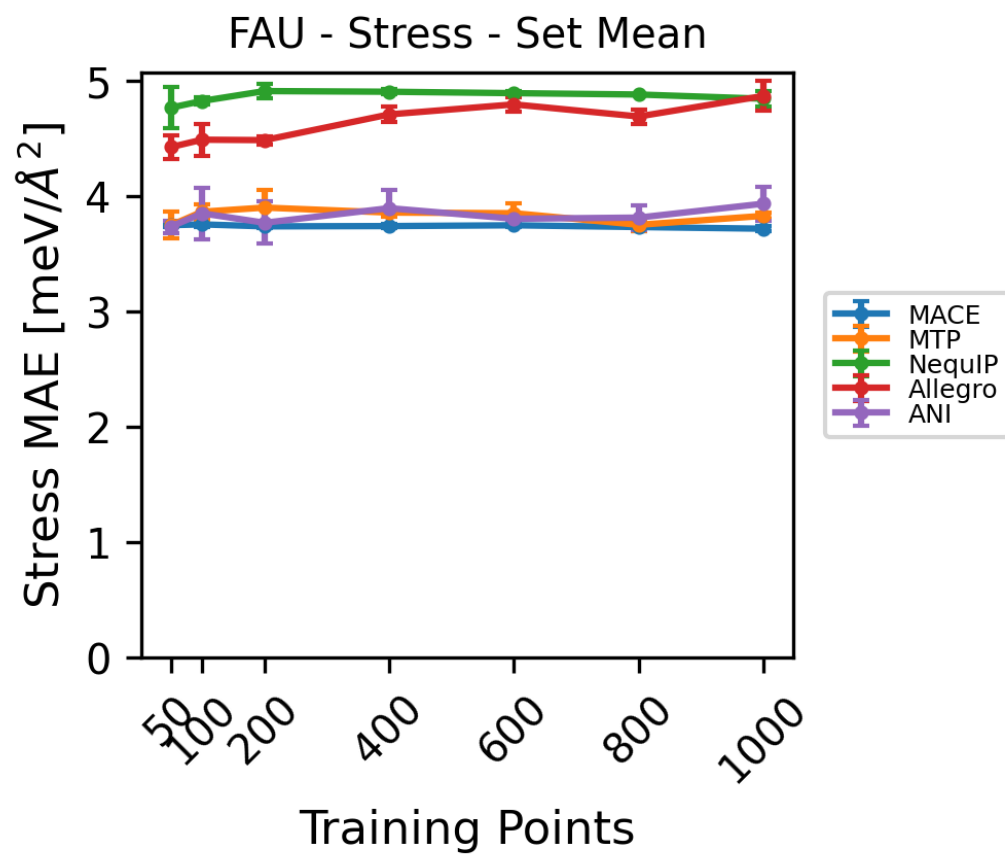
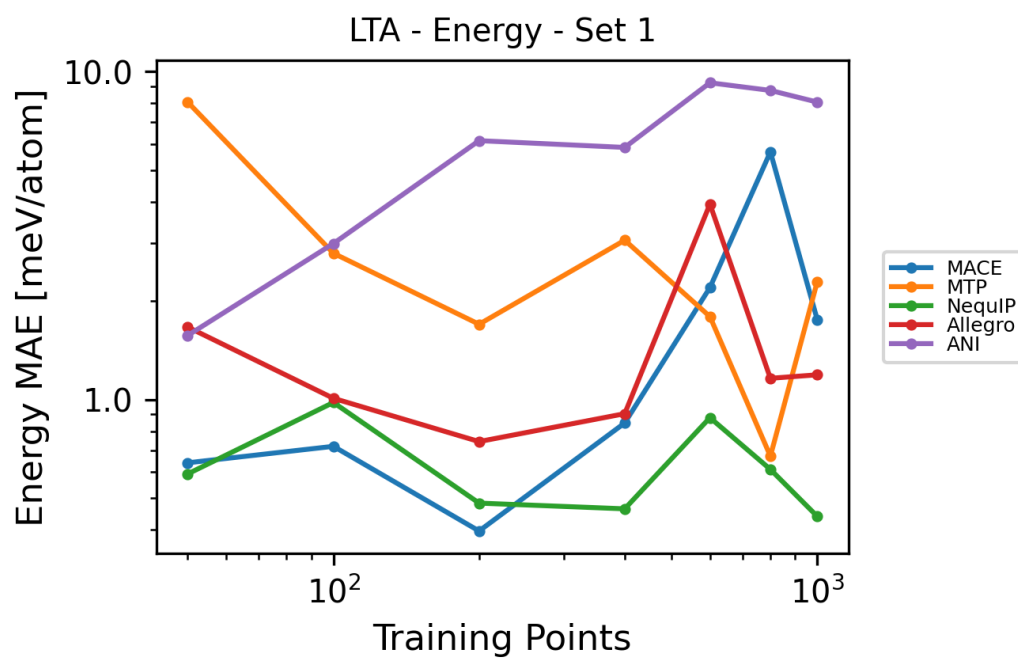**Figure S126.** Force mean absolute error vs training points for FAU, Set mean. Unit: meV/Å.

Figure S127. Stress mean absolute error vs training points for FAU, Set mean. Unit: meV/Å².

Figure S128. Stress mean absolute error vs training points for FAU, Set mean. Unit: meV/Å².
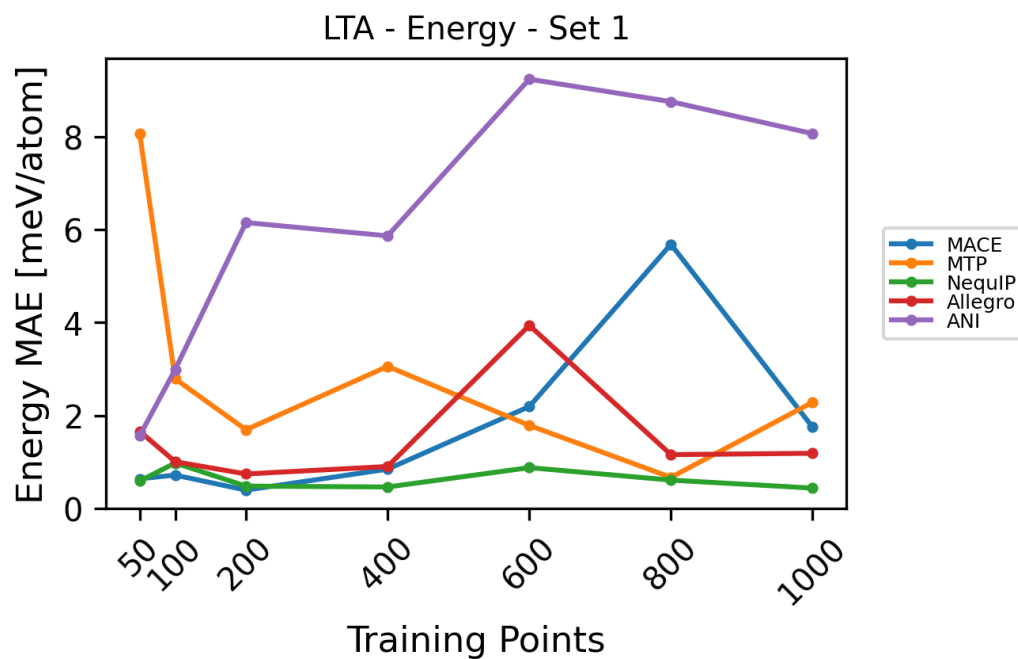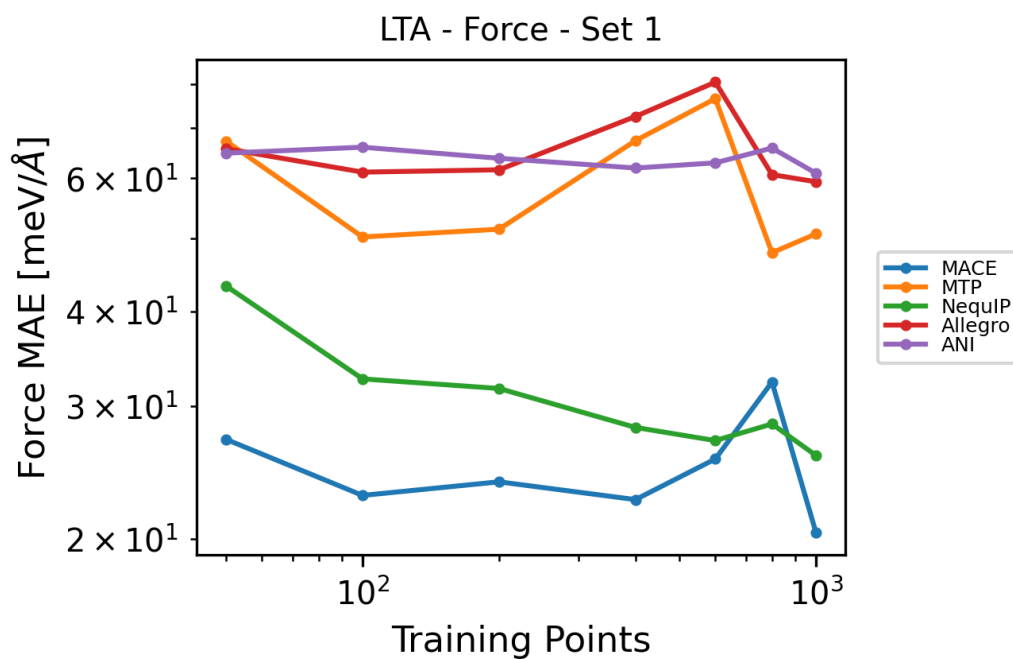
LTA

Figure S129. Energy mean absolute error vs training points for LTA, Set 1. Unit: meV/atom.

Figure S130. Energy mean absolute error vs training points for LTA, Set 1. Unit: meV/atom.

Figure S131. Force mean absolute error vs training points for LTA, Set 1. Unit: meV/Å.

Figure S132. Force mean absolute error vs training points for LTA, Set 1. Unit: meV/Å.

Figure S133. Stress mean absolute error vs training points for LTA, Set 1. Unit: meV/Å².

Figure S134. Stress mean absolute error vs training points for LTA, Set 1. Unit: meV/Å².

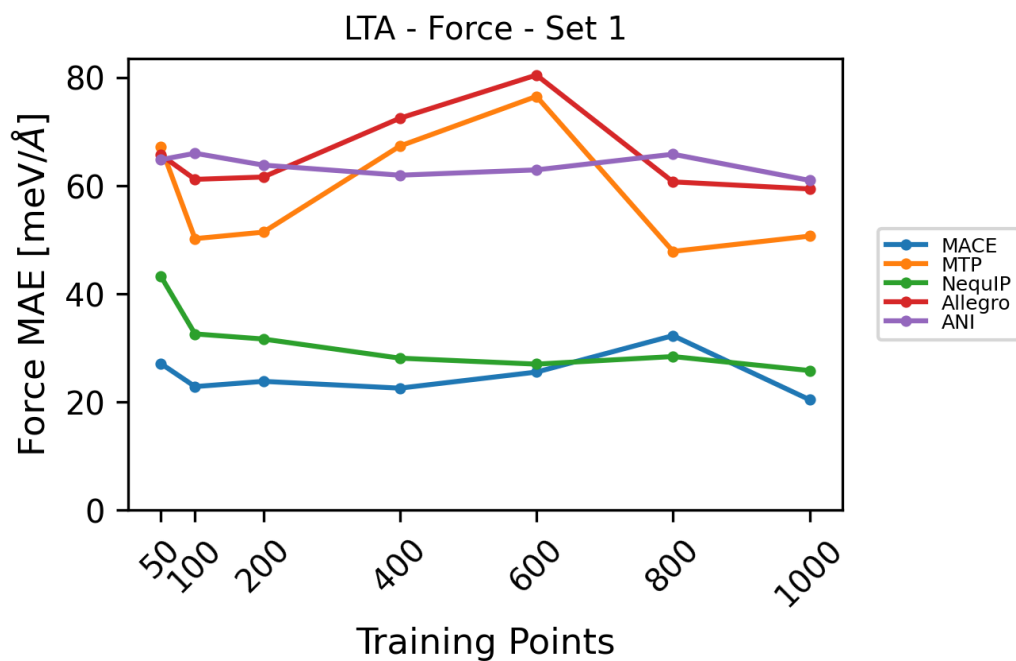**Figure S135.** Energy mean absolute error vs training points for LTA, Set 2. Unit: meV/atom.

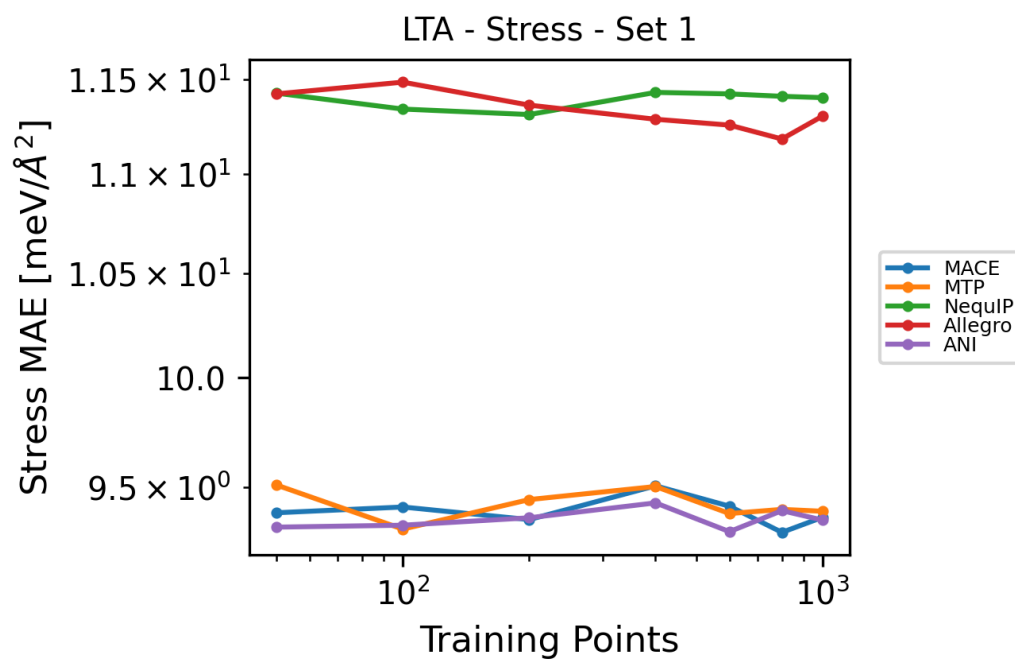**Figure S136.** Energy mean absolute error vs training points for LTA, Set 2. Unit: meV/atom.

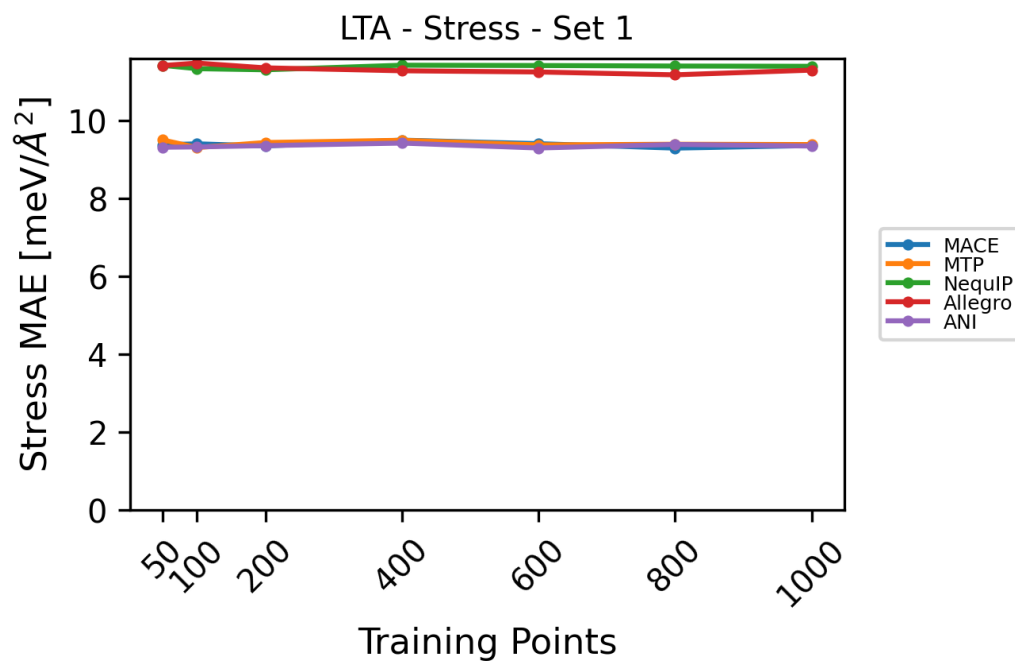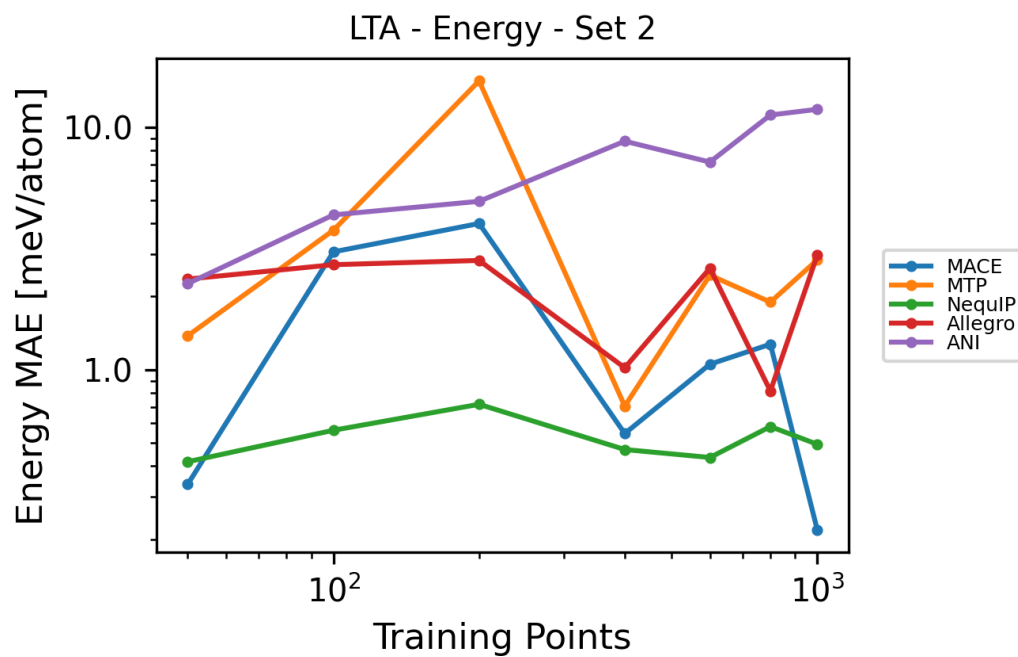**Figure S137.** Force mean absolute error vs training points for LTA, Set 2. Unit: meV/Å.

Figure S138. Force mean absolute error vs training points for LTA, Set 2. Unit: meV/Å.
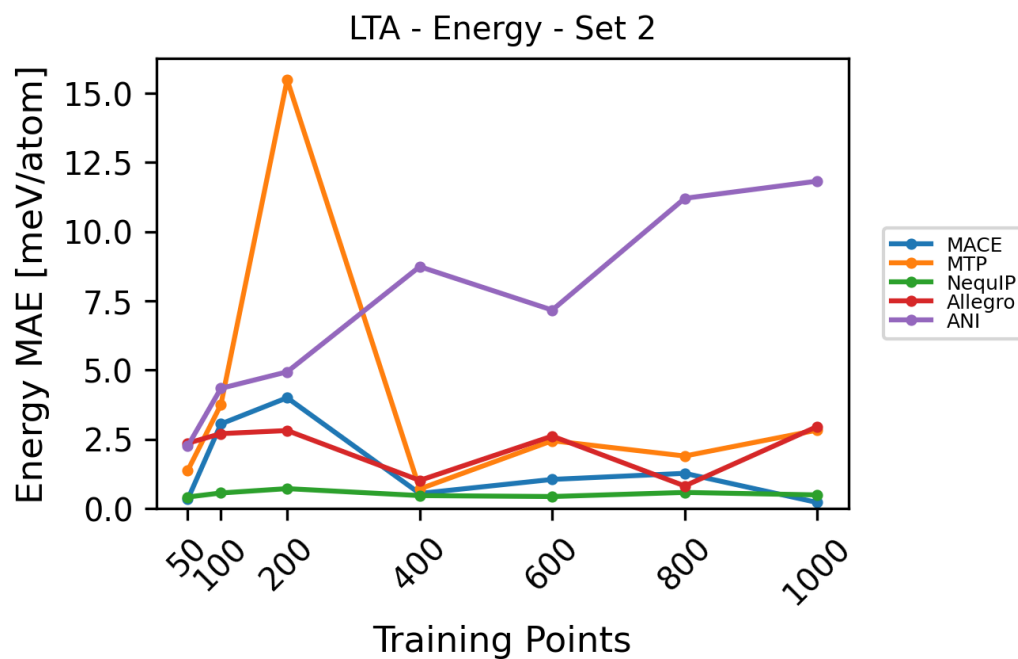
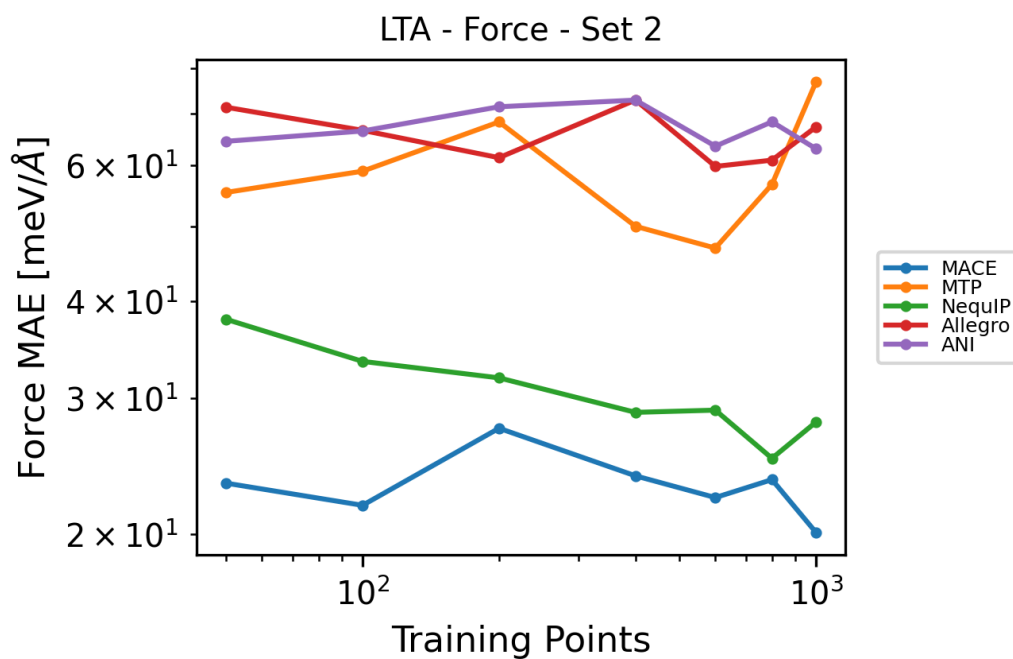**Figure S139.** Stress mean absolute error vs training points for LTA, Set 2. Unit: meV/Å².

Figure S140. Stress mean absolute error vs training points for LTA, Set 2. Unit: meV/Å².
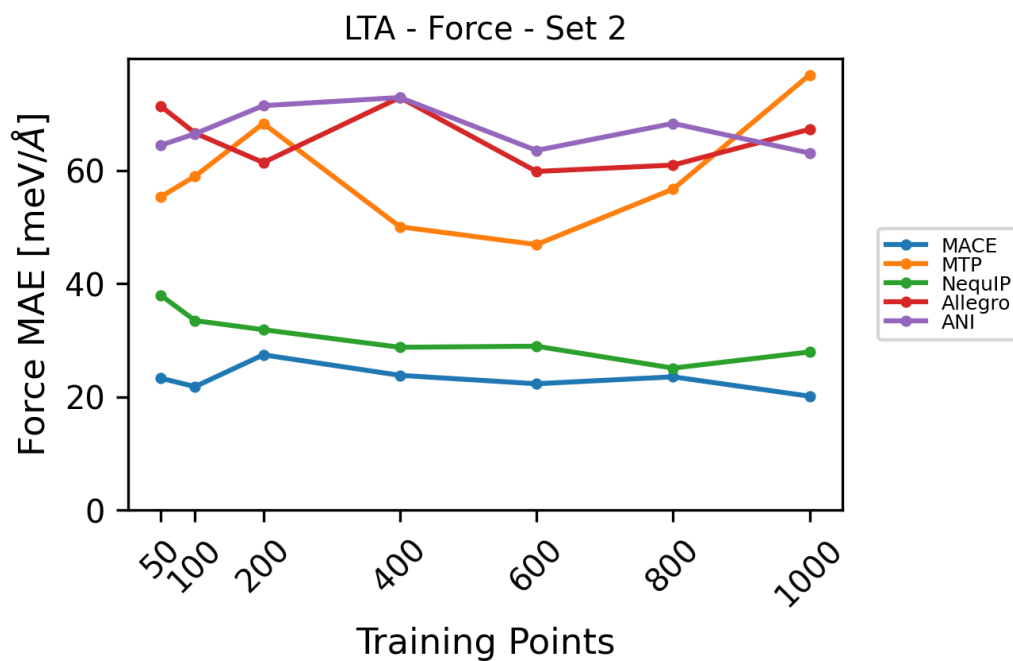
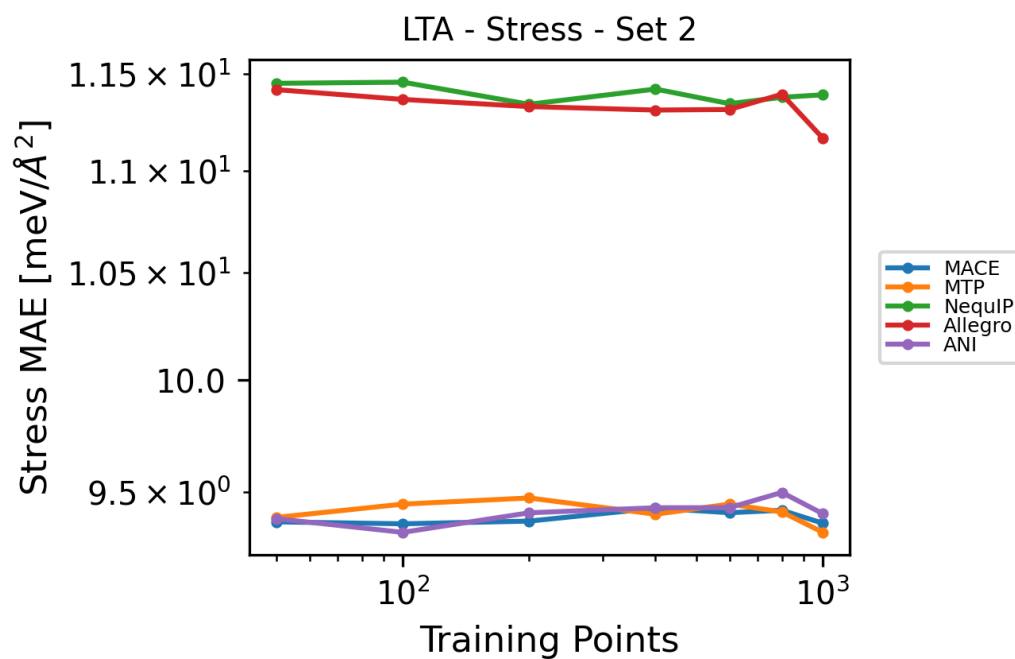**Figure S141.** Energy mean absolute error vs training points for LTA, Set 3. Unit: meV/atom.

Figure S142. Energy mean absolute error vs training points for LTA, Set 3. Unit: meV/atom.

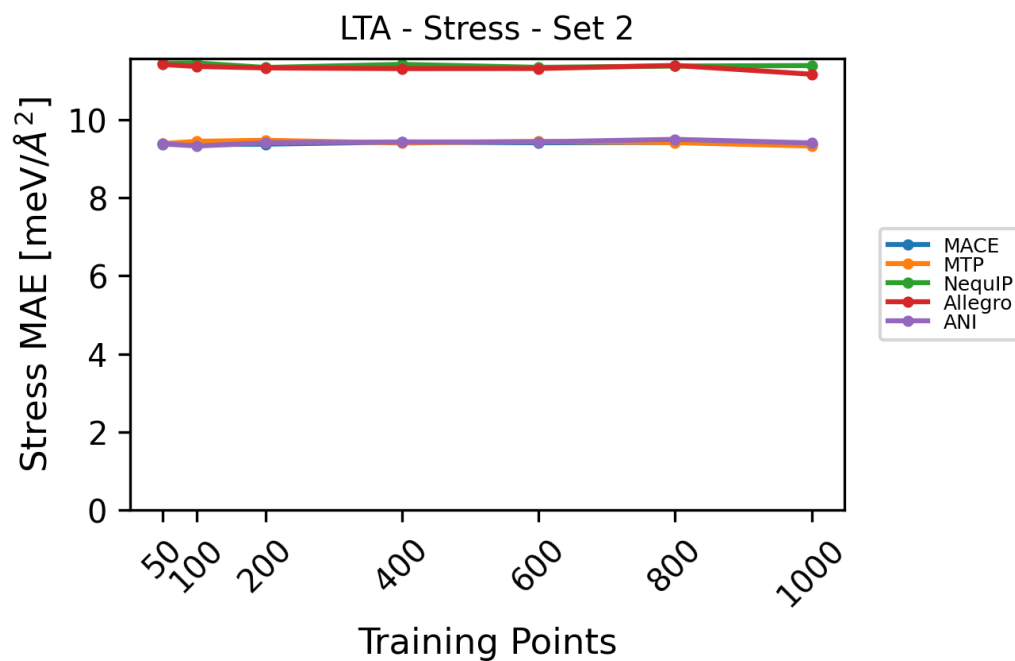**Figure S143.** Force mean absolute error vs training points for LTA, Set 3. Unit: meV/Å.

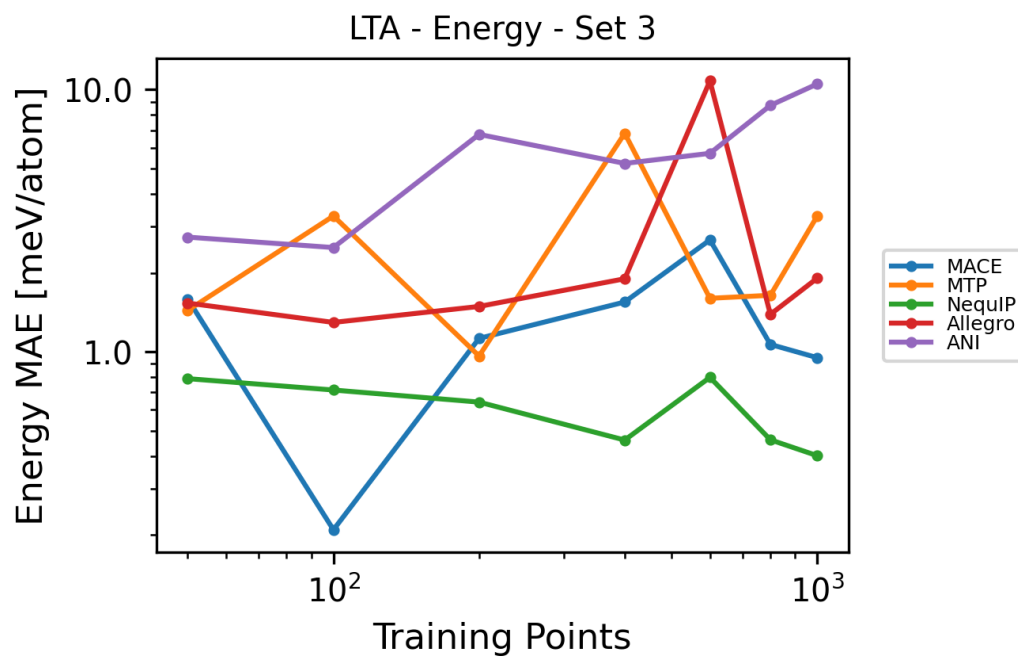**Figure S144.** Force mean absolute error vs training points for LTA, Set 3. Unit: meV/Å.

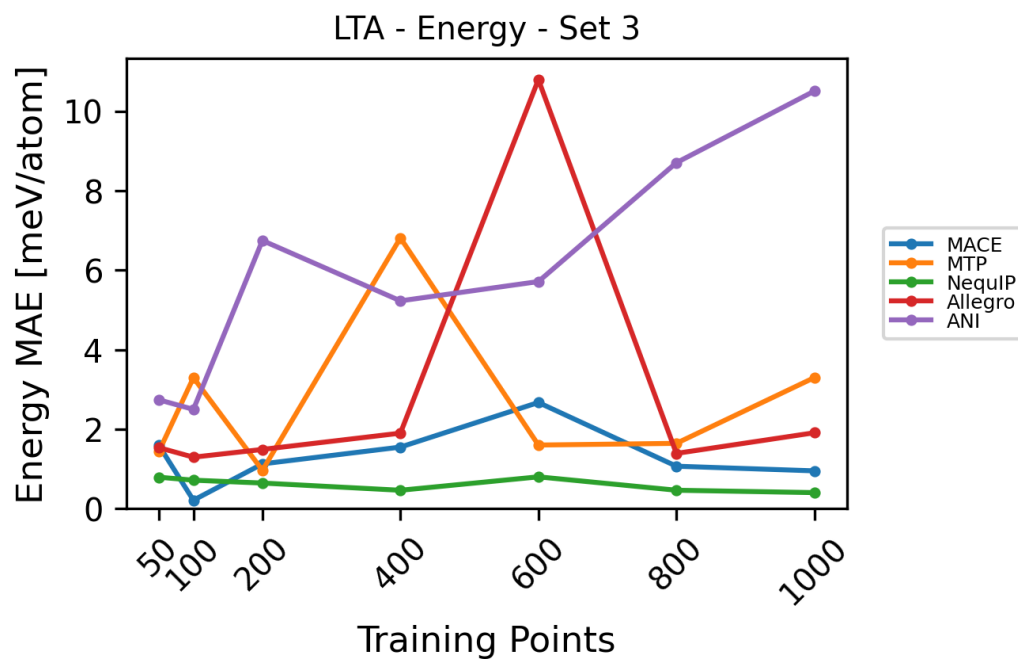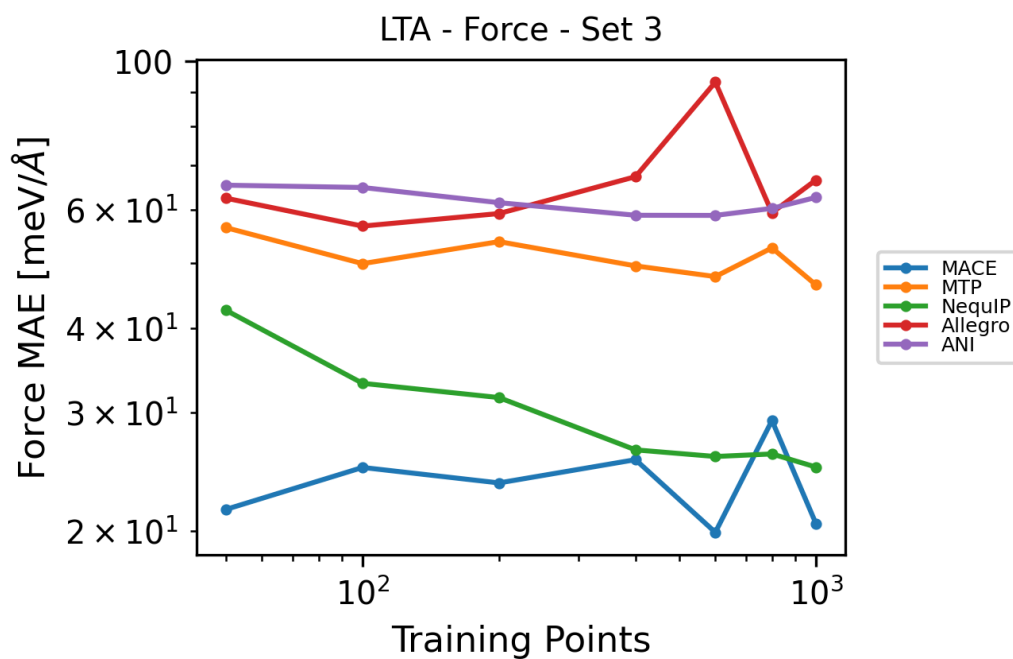**Figure S145.** Stress mean absolute error vs training points for LTA, Set 3. Unit: meV/Å².

Figure S146. Stress mean absolute error vs training points for LTA, Set 3. Unit: meV/Å².
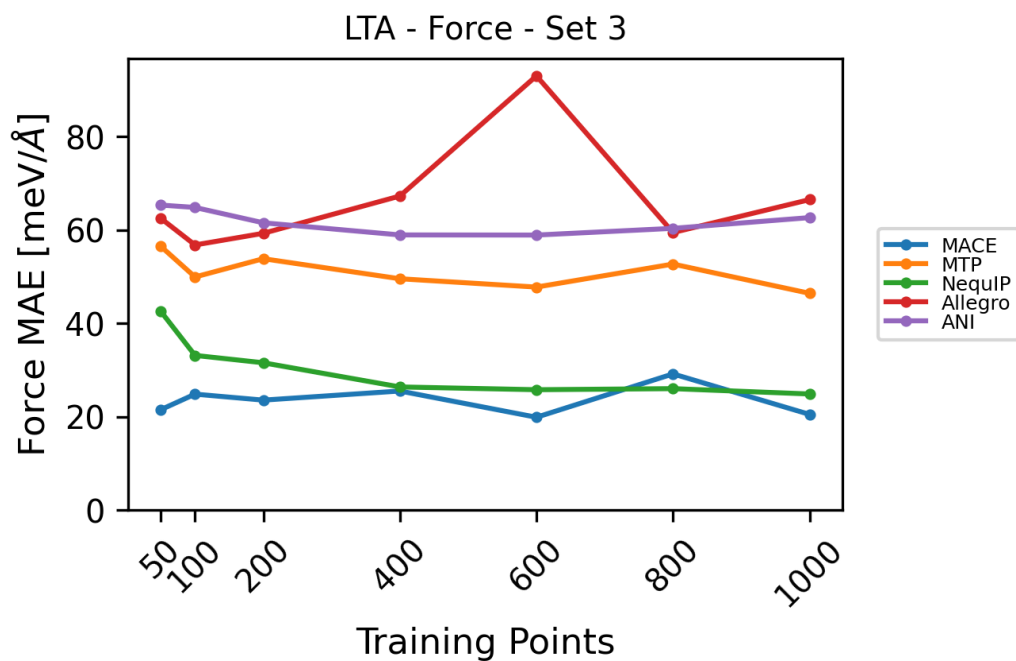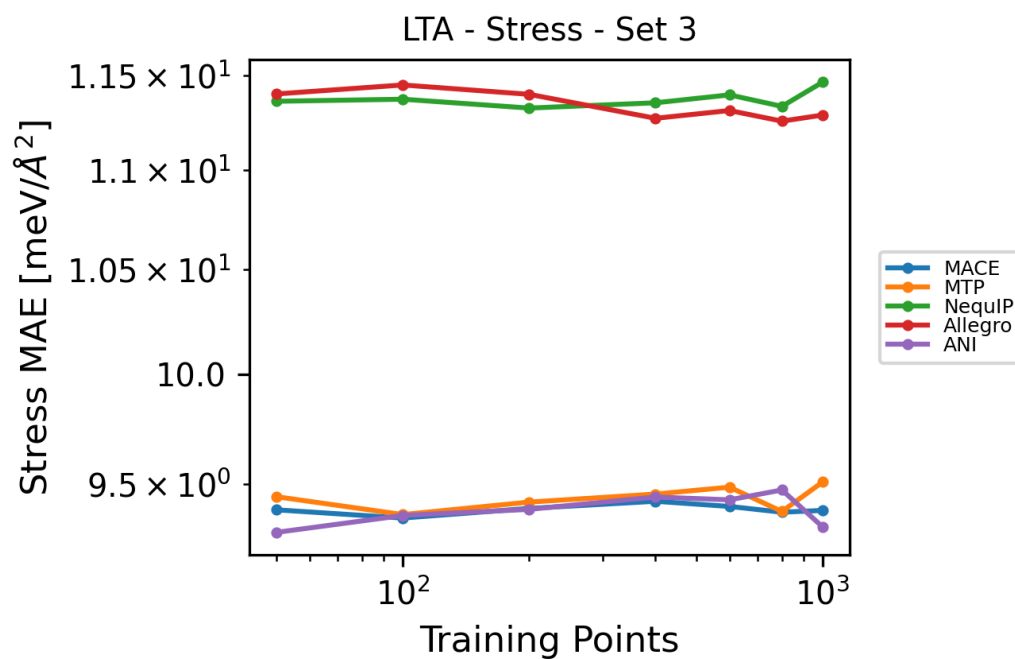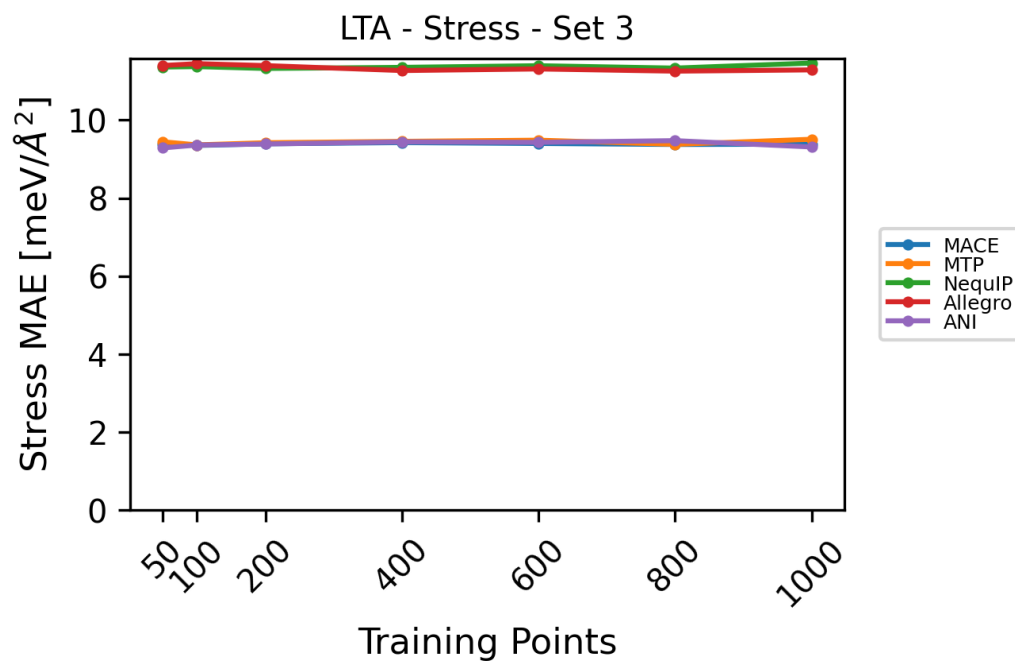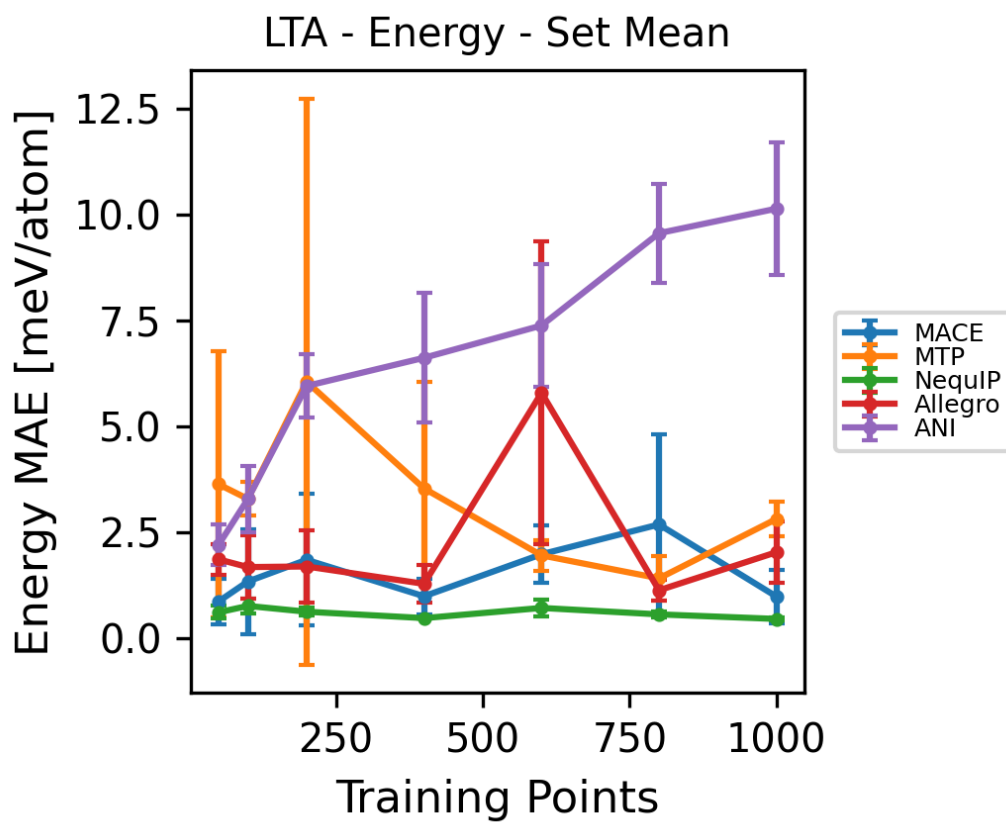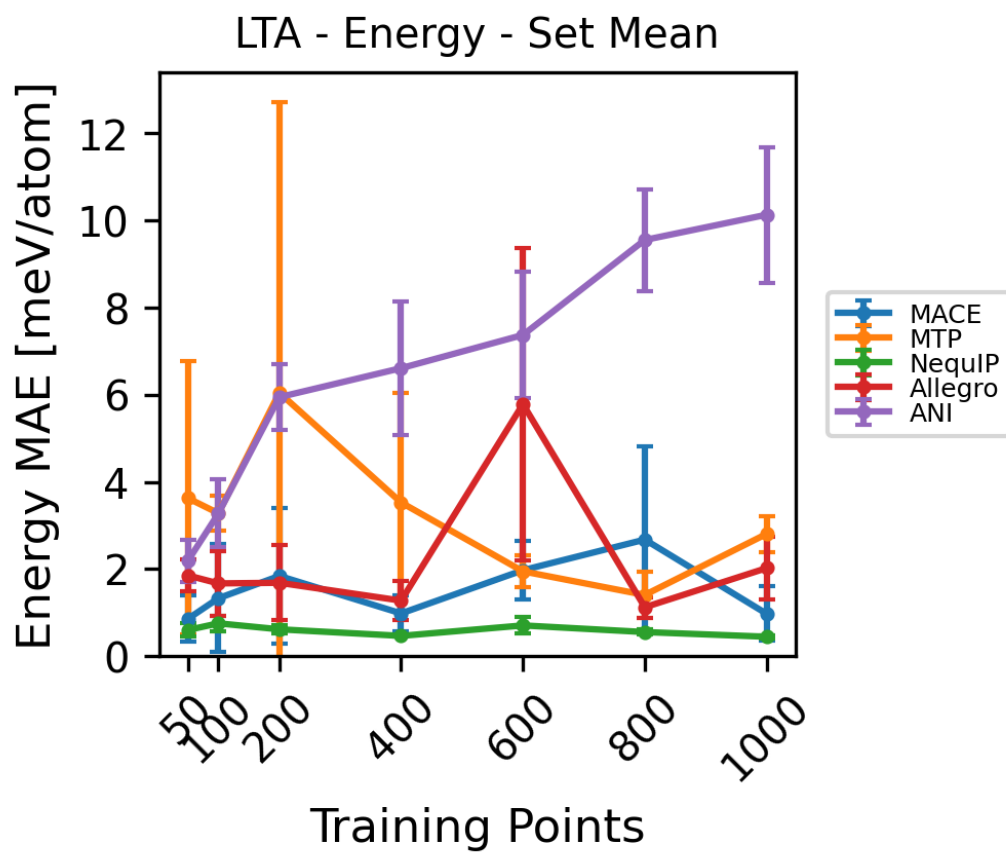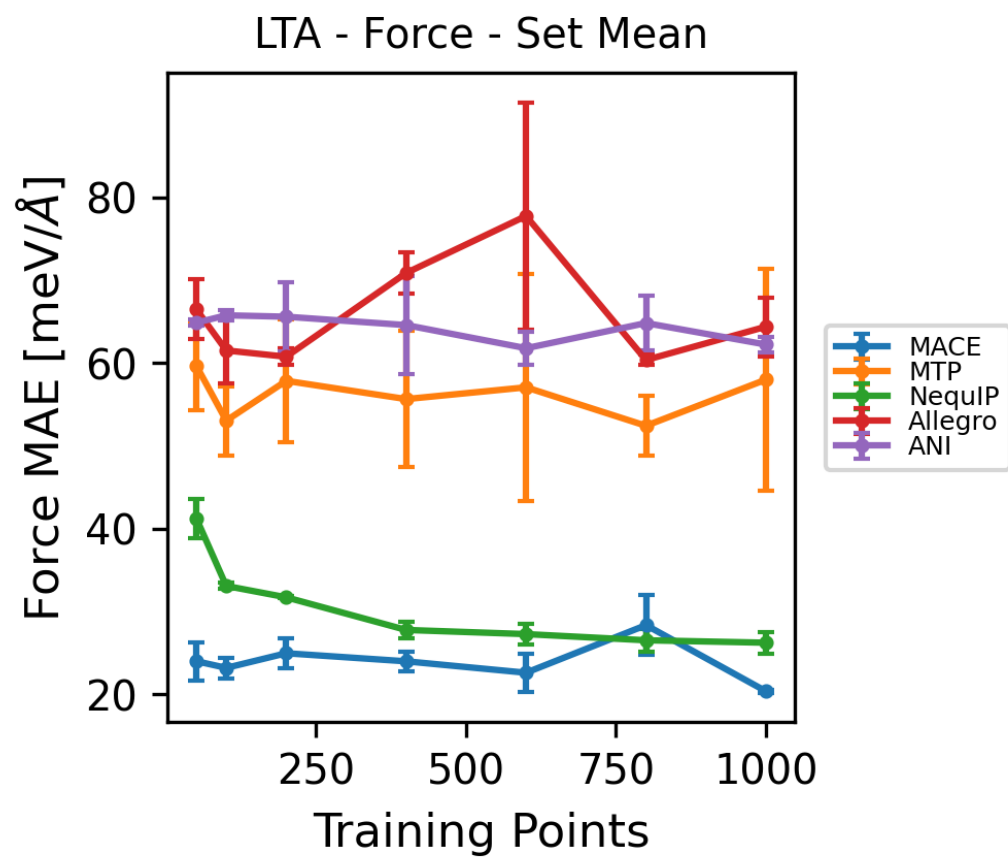
Figure S147. Energy mean absolute error vs training points for LTA, Set mean. Unit: meV/atom.
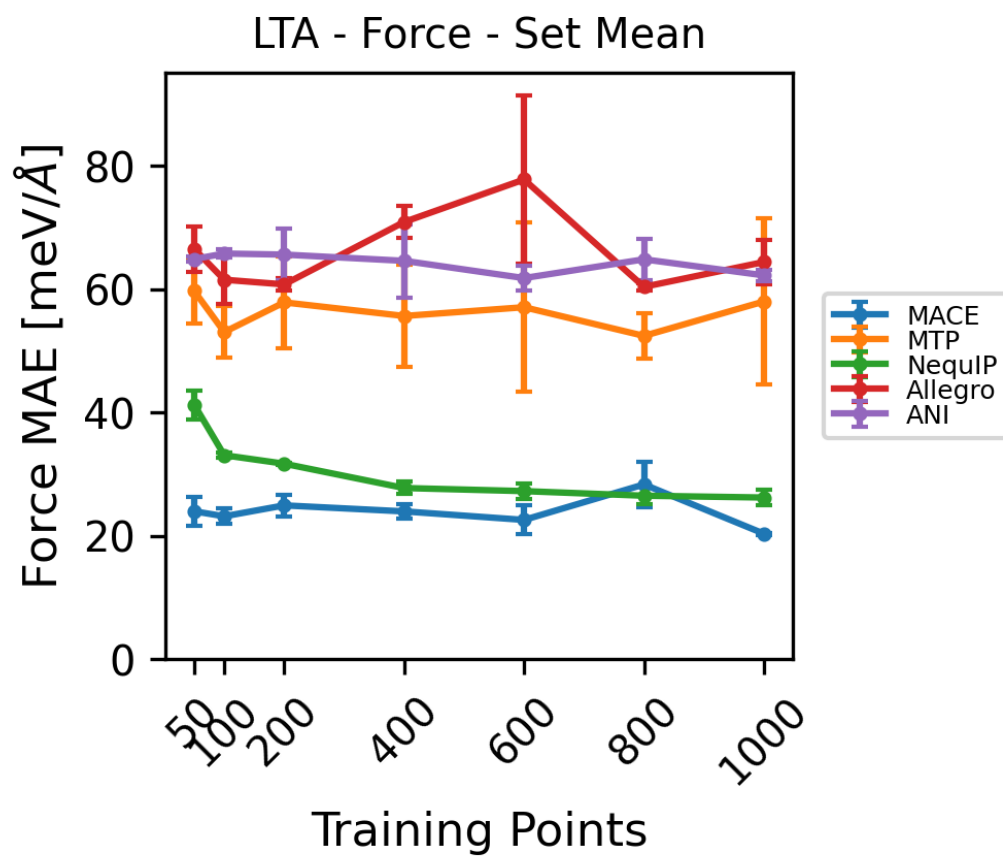
Figure S148. Energy mean absolute error vs training points for LTA, Set mean. Unit: meV/atom.

Figure S149. Force mean absolute error vs training points for LTA, Set mean. Unit: meV/Å.

Figure S150. Force mean absolute error vs training points for LTA, Set mean. Unit: meV/Å.

Figure S151. Stress mean absolute error vs training points for LTA, Set mean. Unit: meV/Å².

Figure S152. Stress mean absolute error vs training points for LTA, Set mean. Unit: meV/Å².

MFI

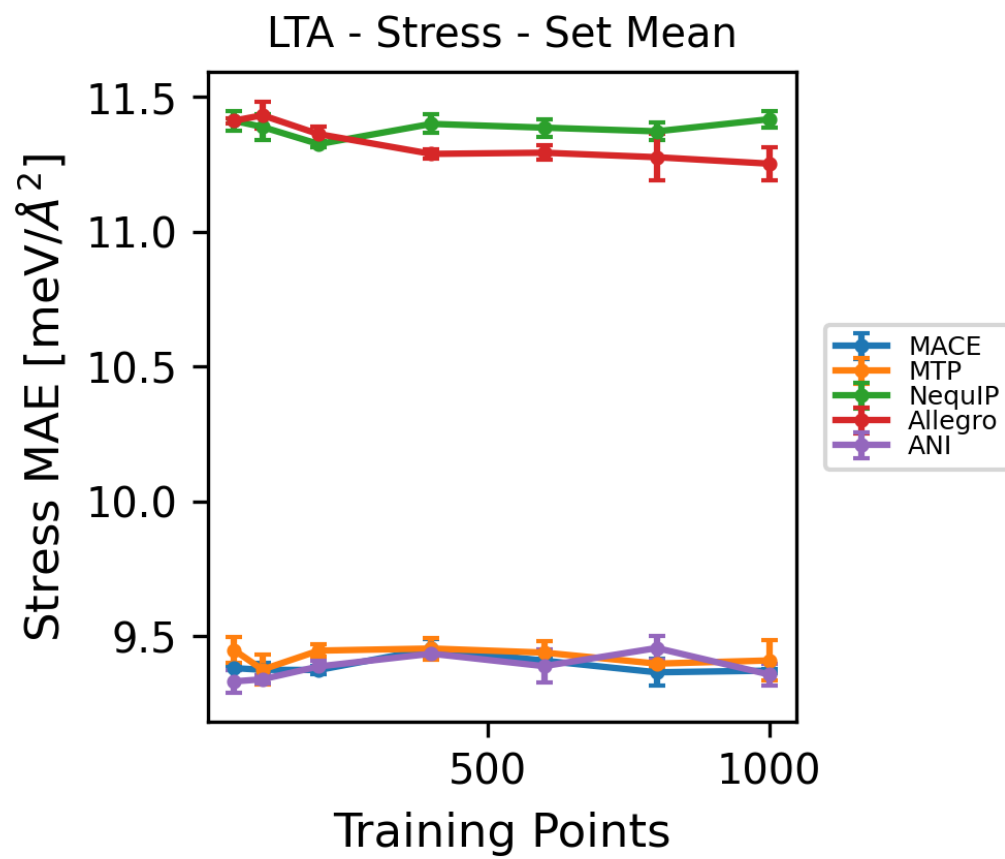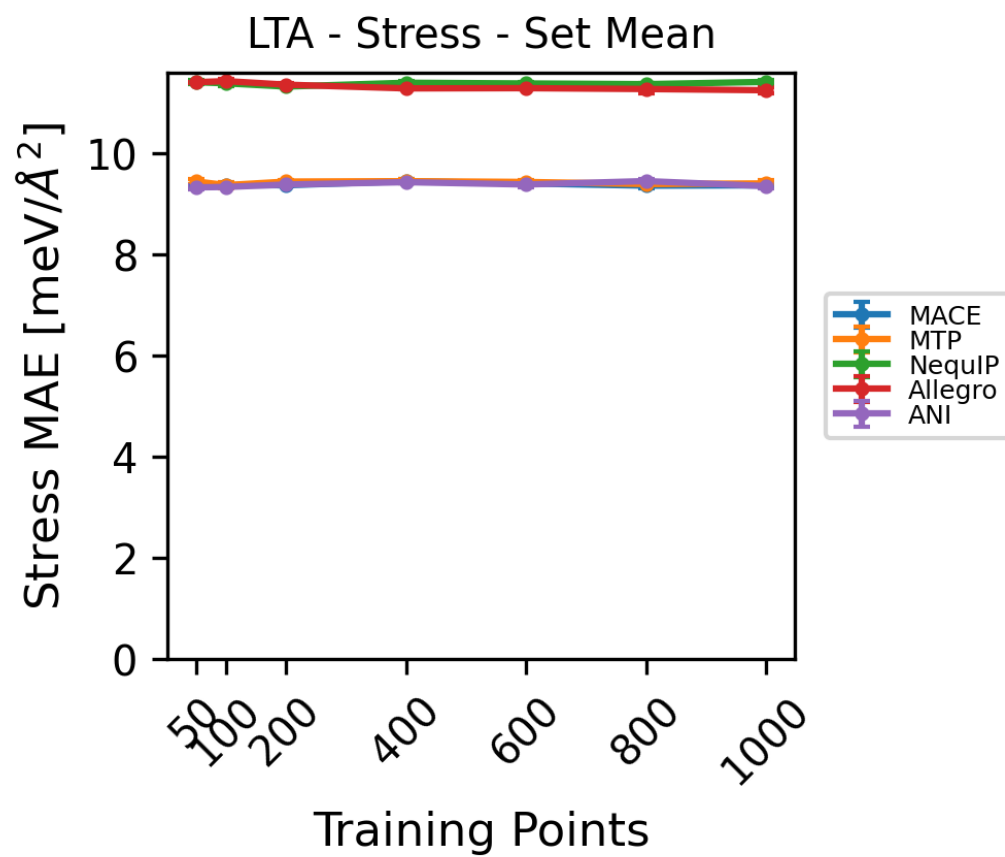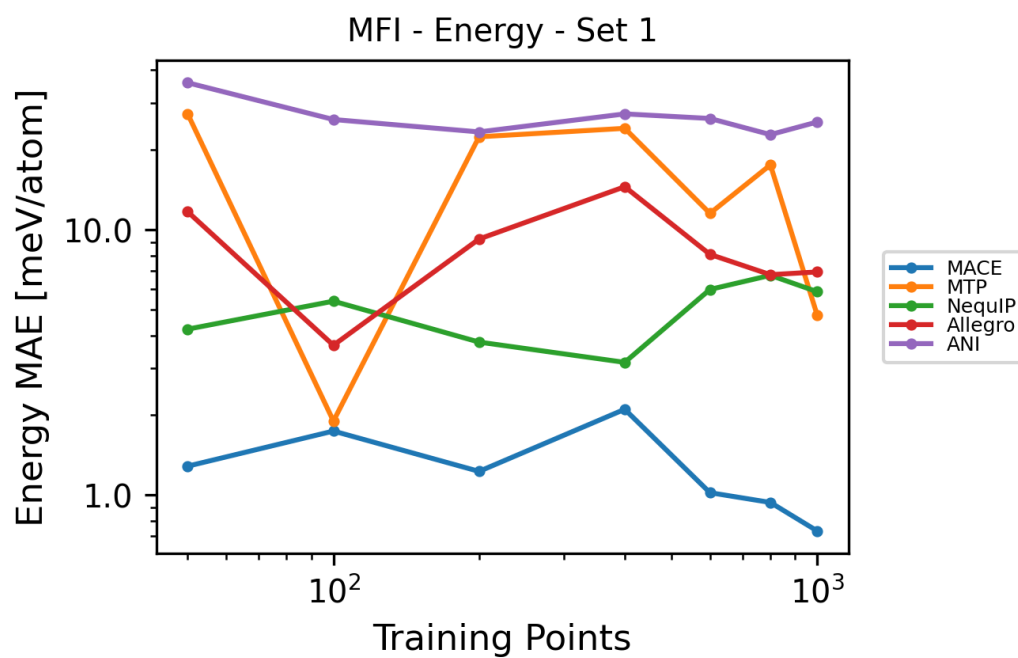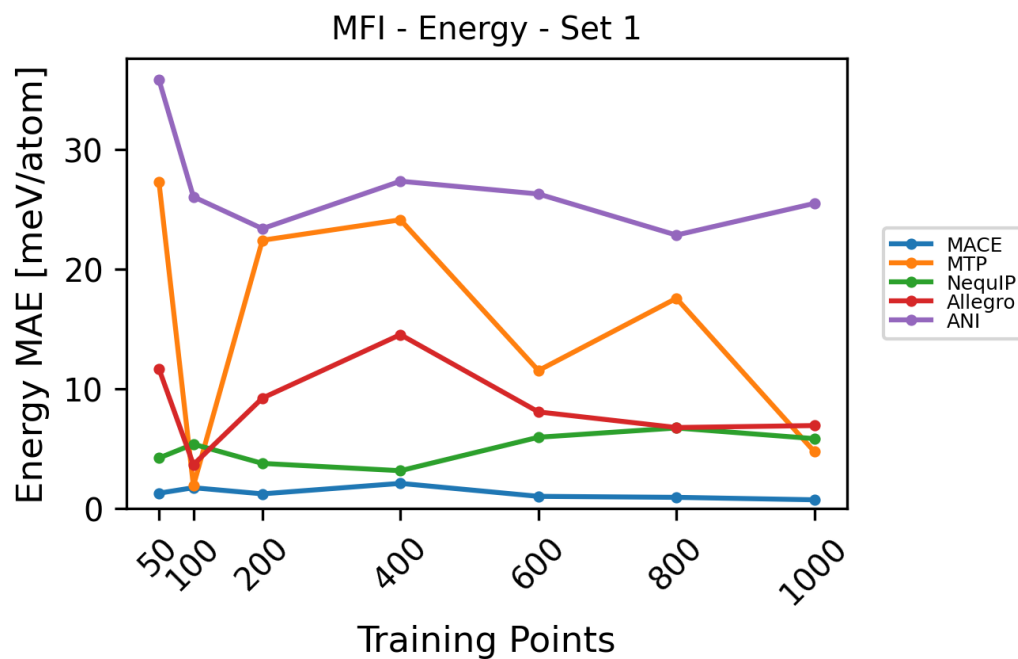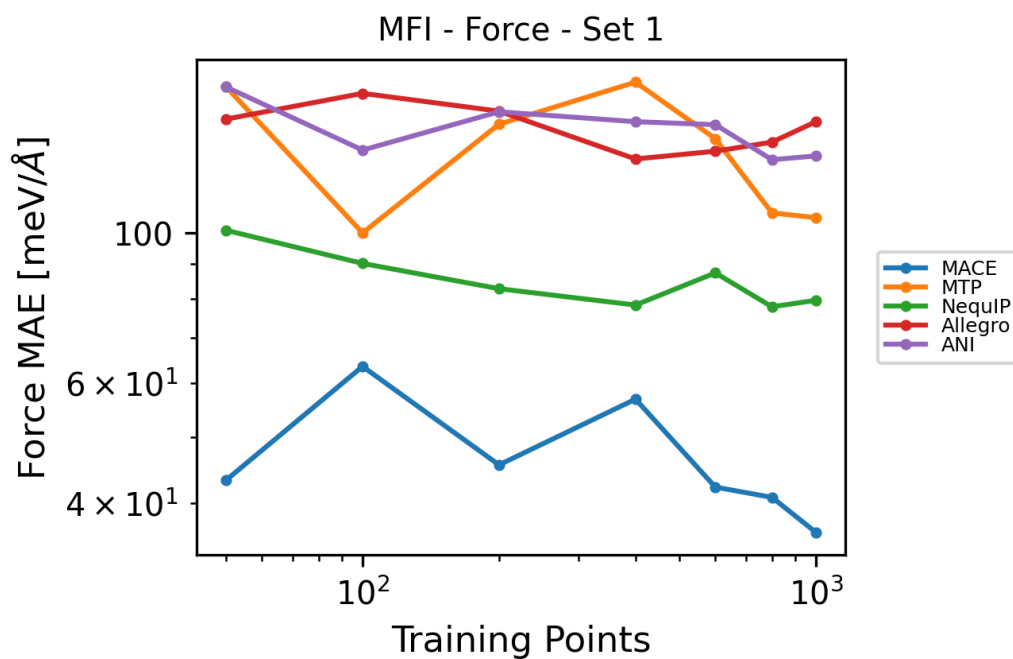**Figure S153.** Energy mean absolute error vs training points for MFI, Set 1. Unit: meV/atom.

Figure S154. Energy mean absolute error vs training points for MFI, Set 1. Unit: meV/atom.

Figure S155. Force mean absolute error vs training points for MFI, Set 1. Unit: meV/Å.

Figure S156. Force mean absolute error vs training points for MFI, Set 1. Unit: meV/Å.

Figure S157. Stress mean absolute error vs training points for MFI, Set 1. Unit: meV/Å².

Figure S158. Stress mean absolute error vs training points for MFI, Set 1. Unit: meV/Å².

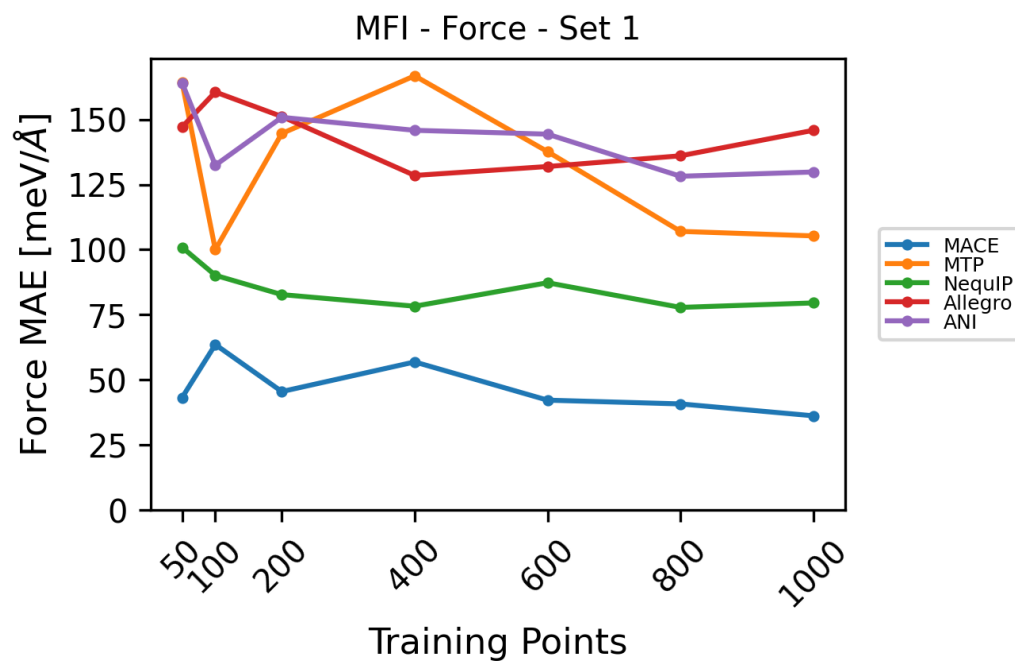**Figure S159.** Energy mean absolute error vs training points for MFI, Set 2. Unit: meV/atom.

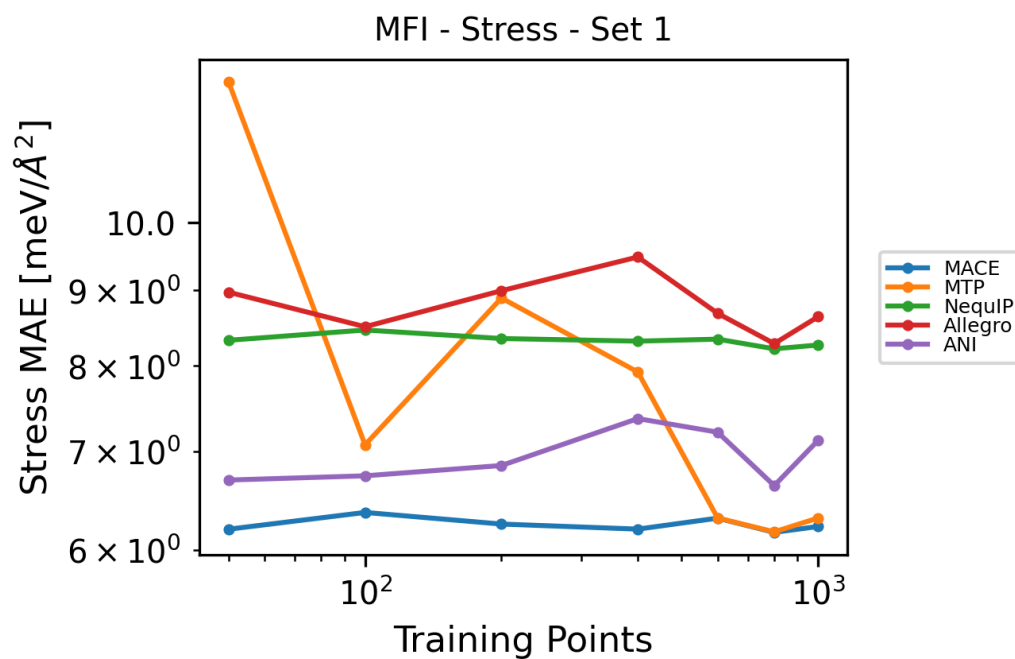**Figure S160.** Energy mean absolute error vs training points for MFI, Set 2. Unit: meV/atom.

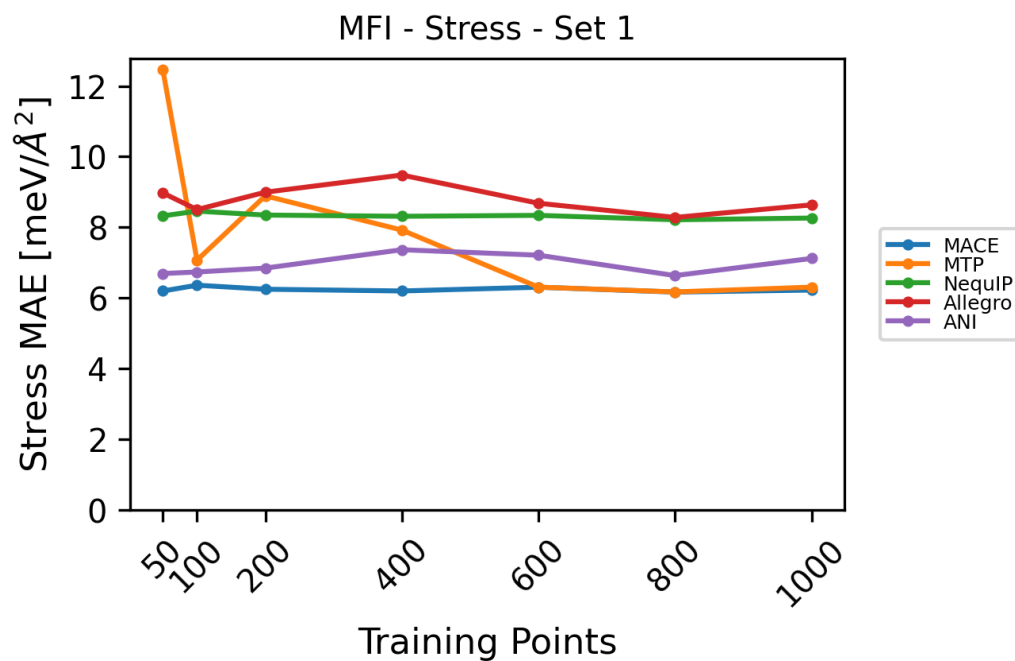**Figure S161.** Force mean absolute error vs training points for MFI, Set 2. Unit: meV/Å.
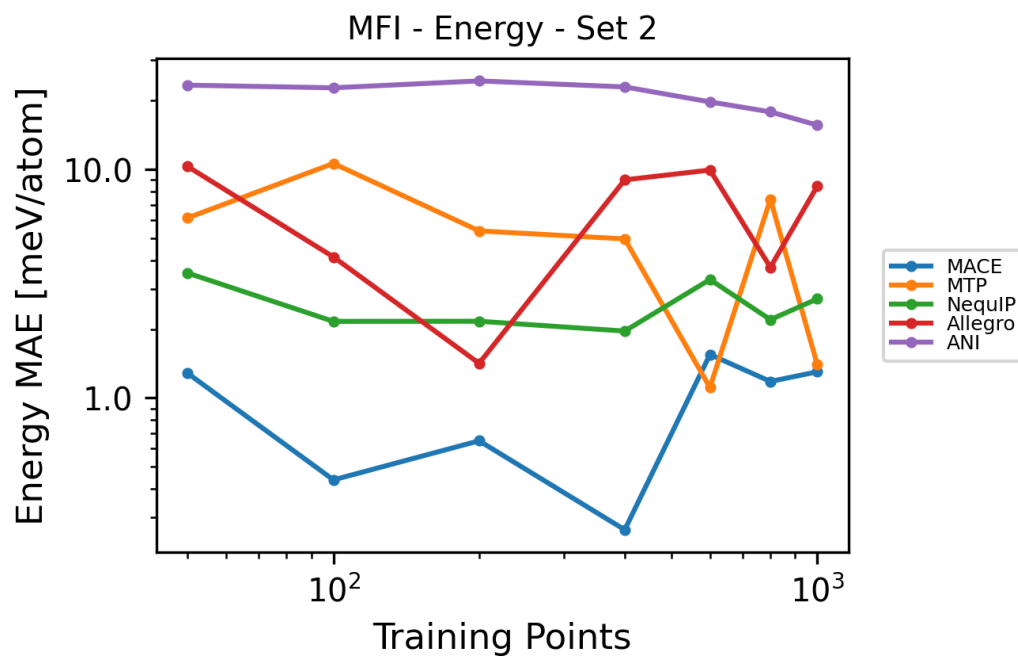
Figure S162. Force mean absolute error vs training points for MFI, Set 2. Unit: meV/Å.
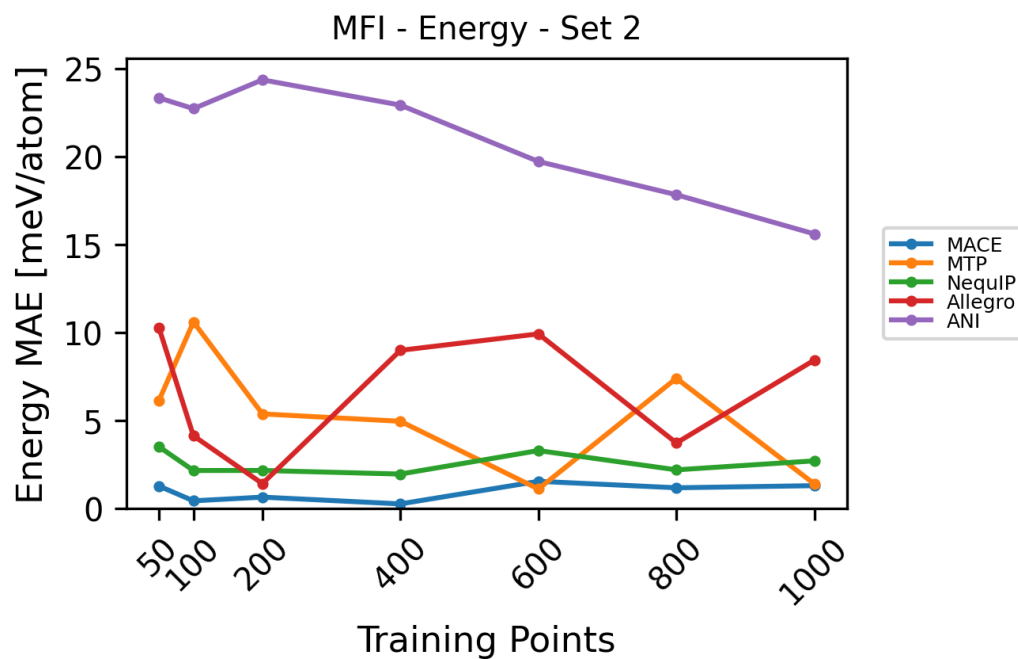
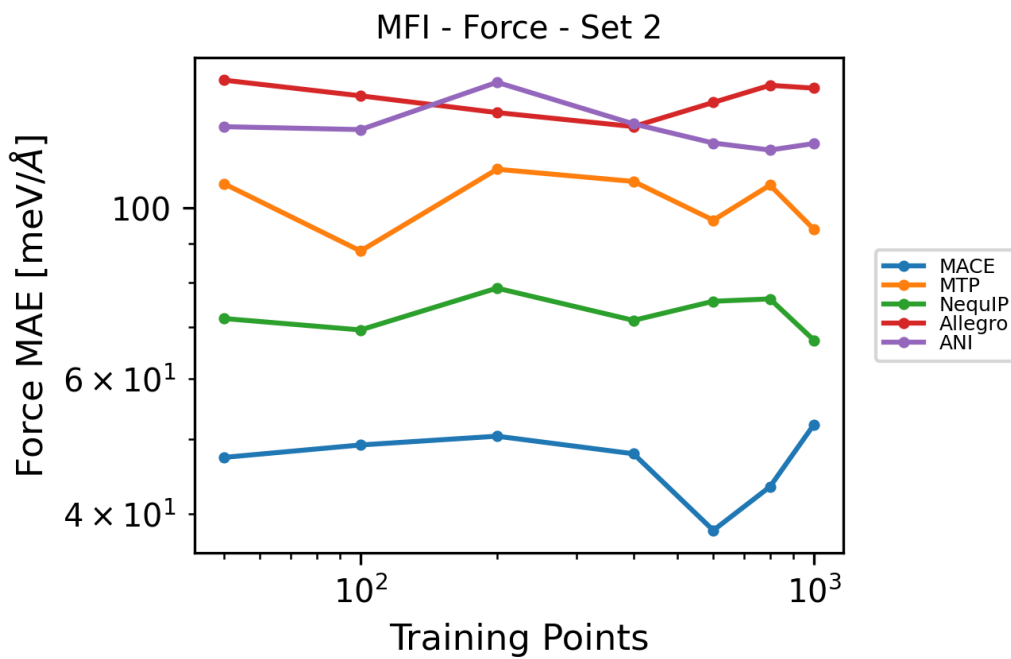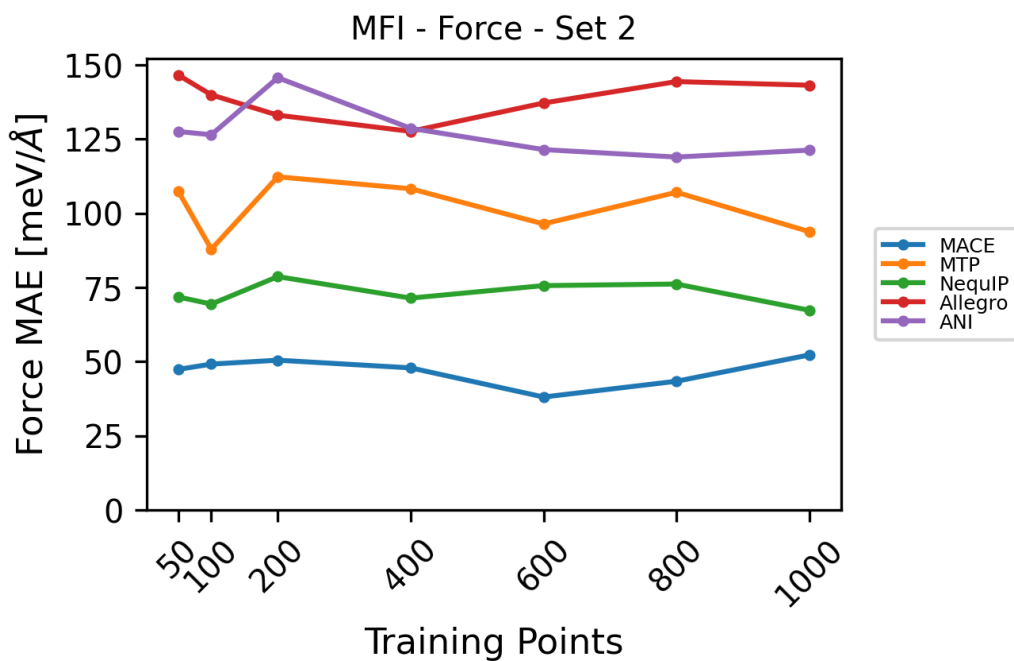**Figure S163.** Stress mean absolute error vs training points for MFI, Set 2. Unit: meV/Å².

Figure S164. Stress mean absolute error vs training points for MFI, Set 2. Unit: meV/Å².

Figure S165. Force mean absolute error vs training points for MFI, Set 3. Unit: meV/Å.

Figure S166. Force mean absolute error vs training points for MFI, Set 3. Unit: meV/Å.

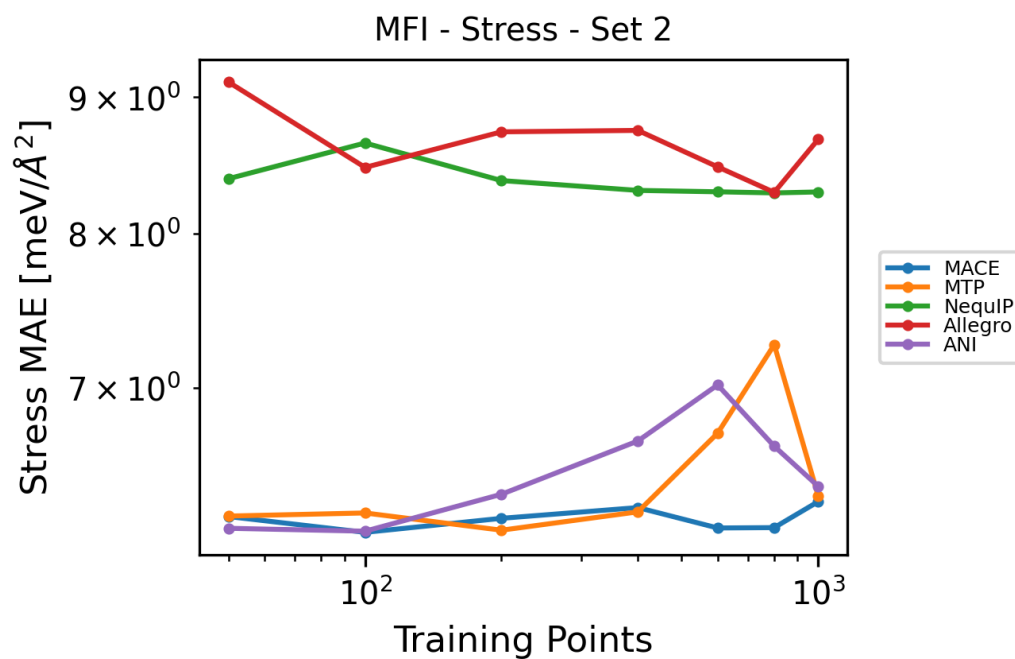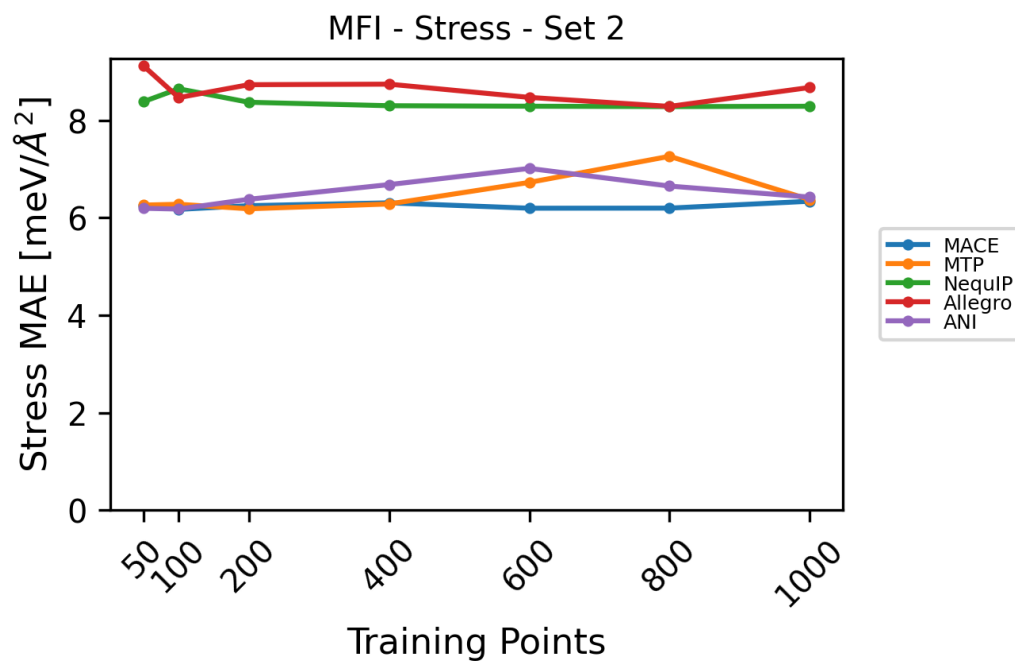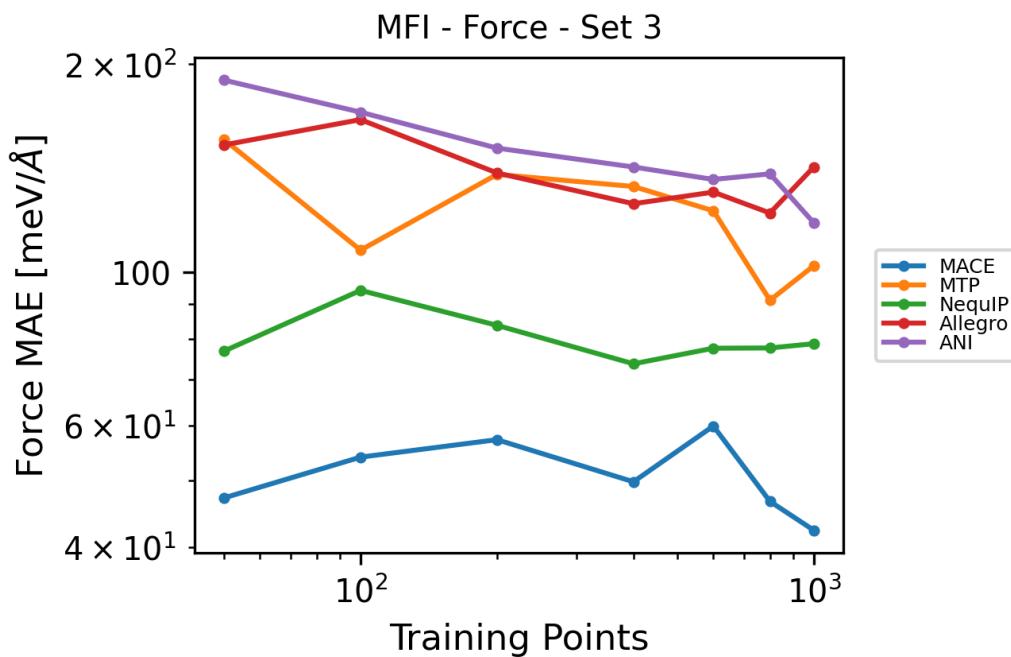**Figure S167.** Stress mean absolute error vs training points for MFI, Set 3. Unit: meV/Å².
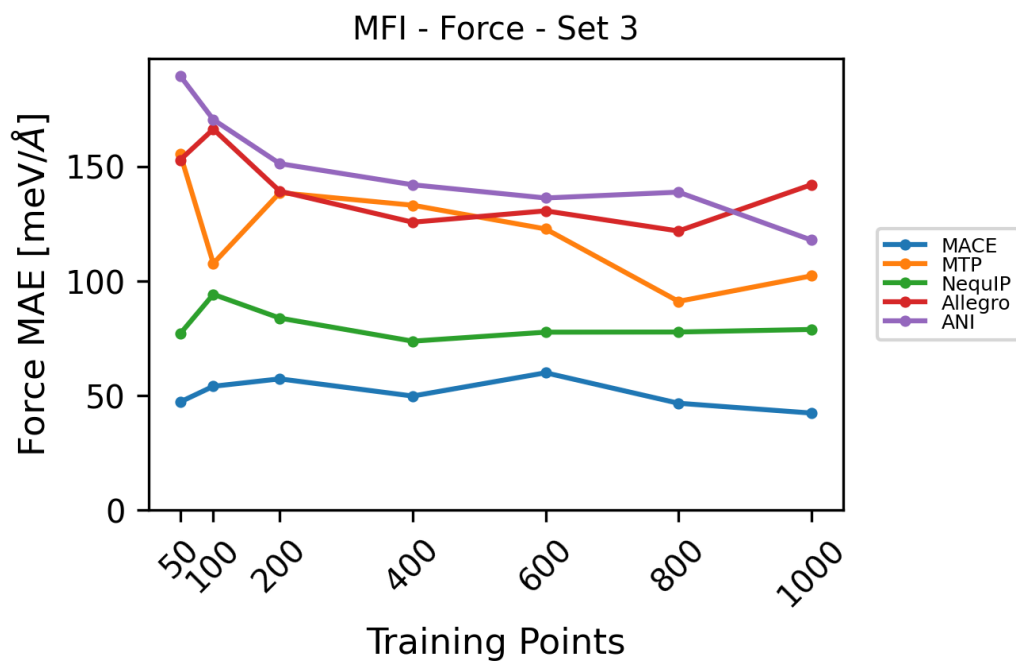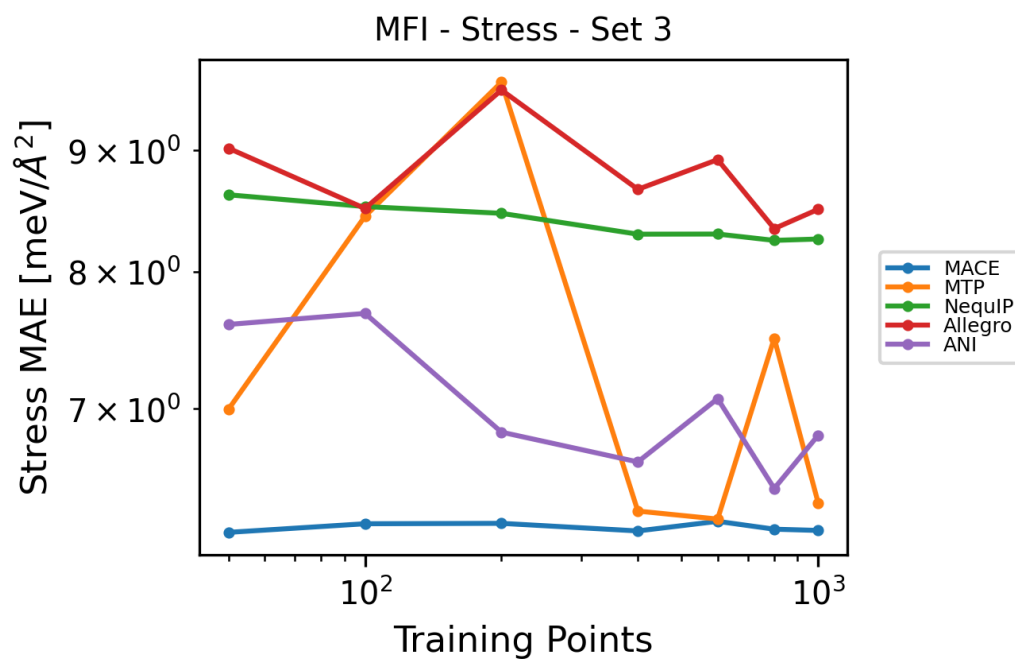
Figure S168. Stress mean absolute error vs training points for MFI, Set 3. Unit: meV/Å².

Figure S169. Force mean absolute error vs training points for MFI, Set mean. Unit: meV/Å.

Figure S170. Force mean absolute error vs training points for MFI, Set mean. Unit: meV/Å.

Figure S171. Stress mean absolute error vs training points for MFI, Set mean. Unit: meV/Å².
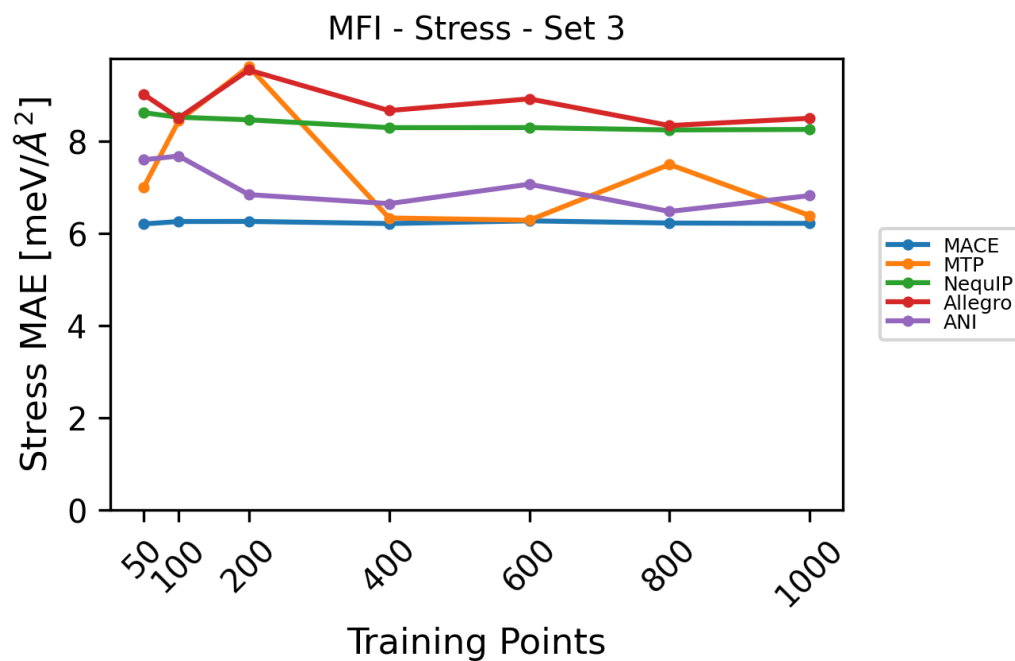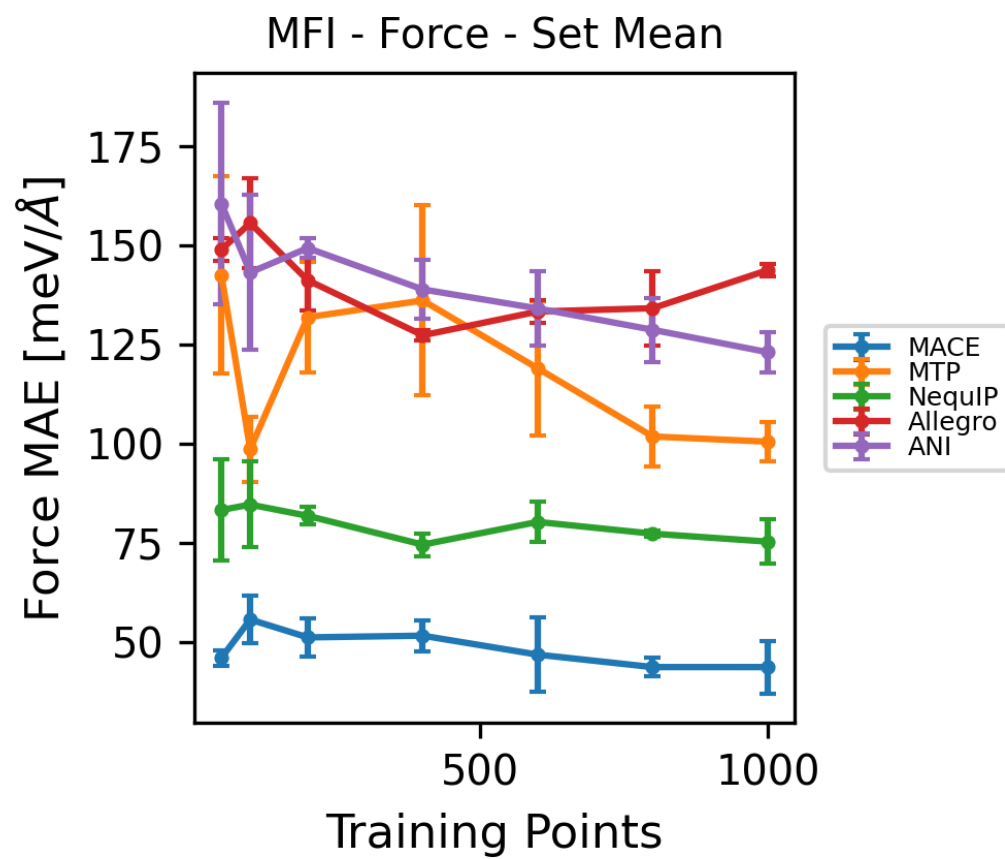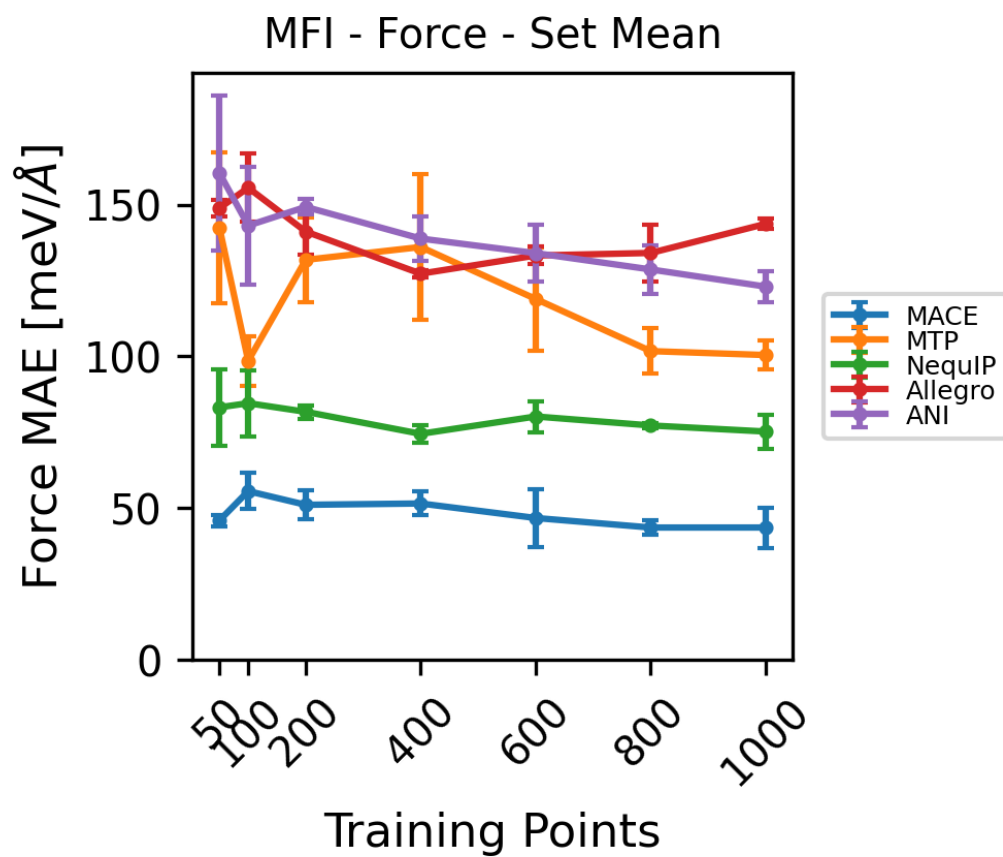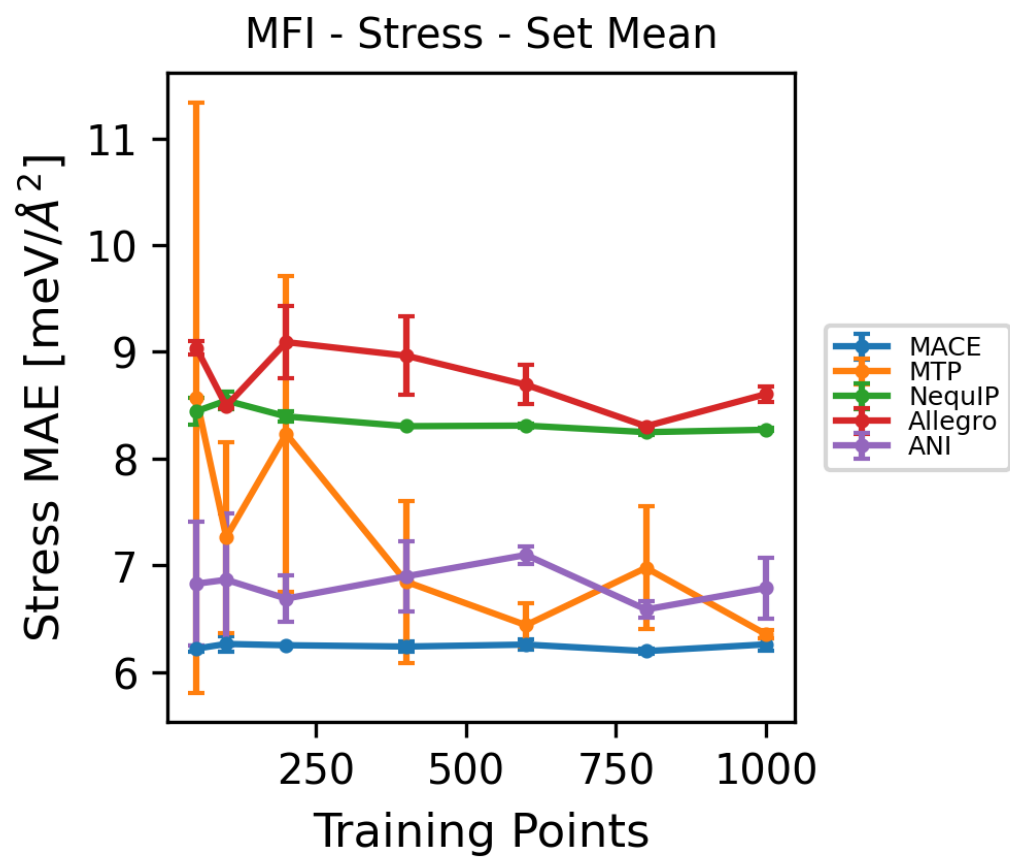
Figure S172. Stress mean absolute error vs training points for MFI, Set mean. Unit: meV/Å².

Reaction

Figure S173. Energy mean absolute error vs training points for Reaction, Set 1. Unit: meV/atom.

Figure S174. Energy mean absolute error vs training points for Reaction, Set 1. Unit: meV/atom.
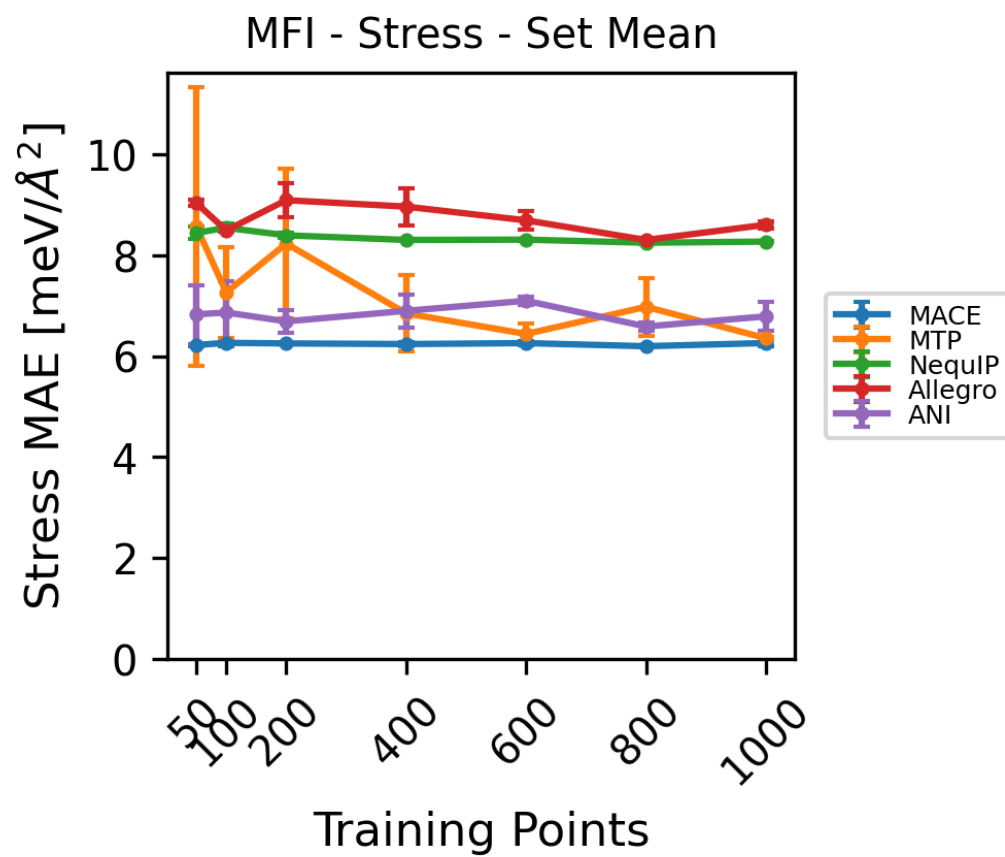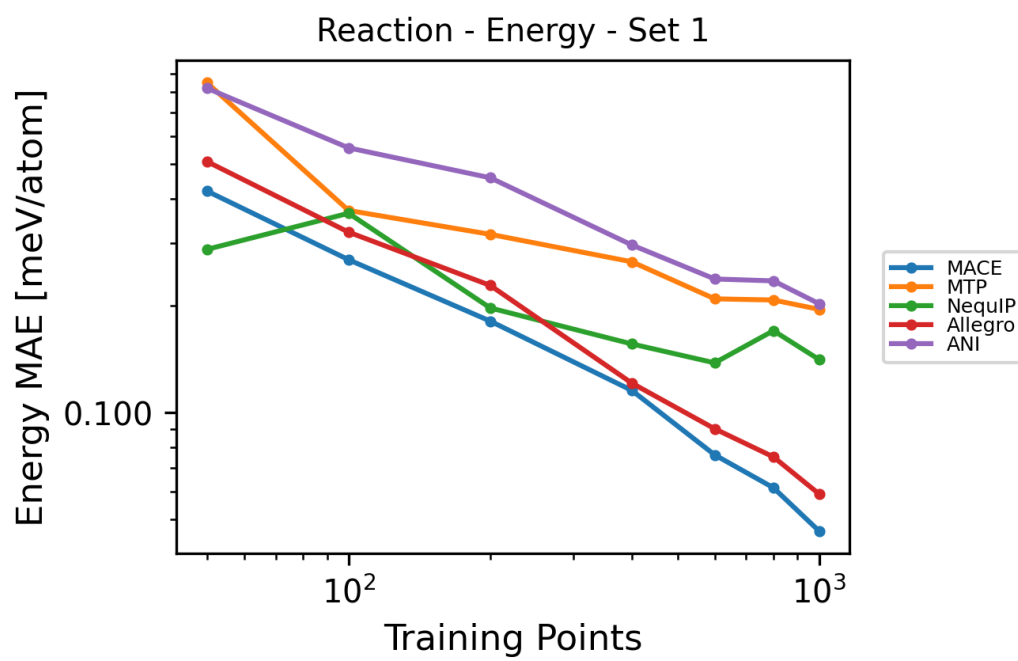
Figure S175. Force mean absolute error vs training points for Reaction, Set 1. Unit: meV/Å.
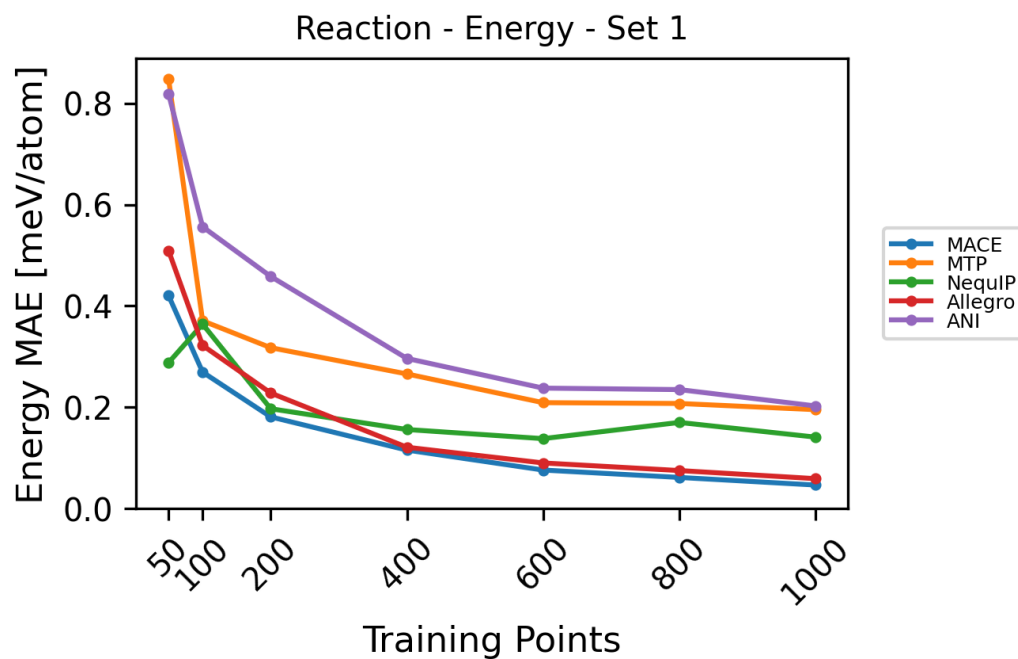
Figure S176. Force mean absolute error vs training points for Reaction, Set 1. Unit: meV/Å.
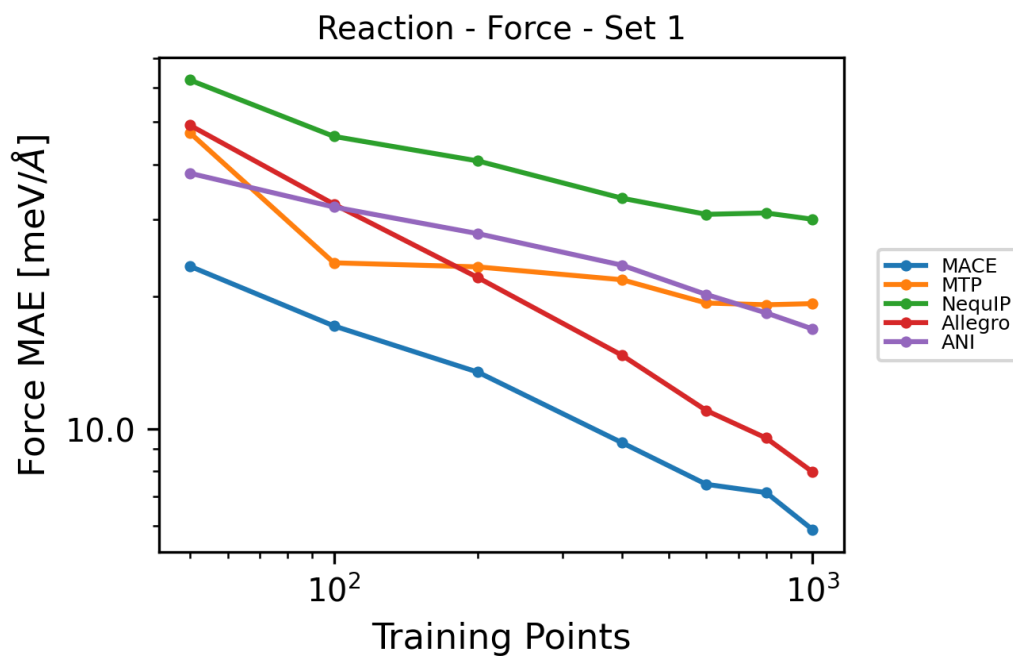
Figure S177. Energy mean absolute error vs training points for Reaction, Set 2. Unit: meV/atom.

Figure S178. Energy mean absolute error vs training points for Reaction, Set 2. Unit: meV/atom.

Figure S179. Force mean absolute error vs training points for Reaction, Set 2. Unit: meV/Å.

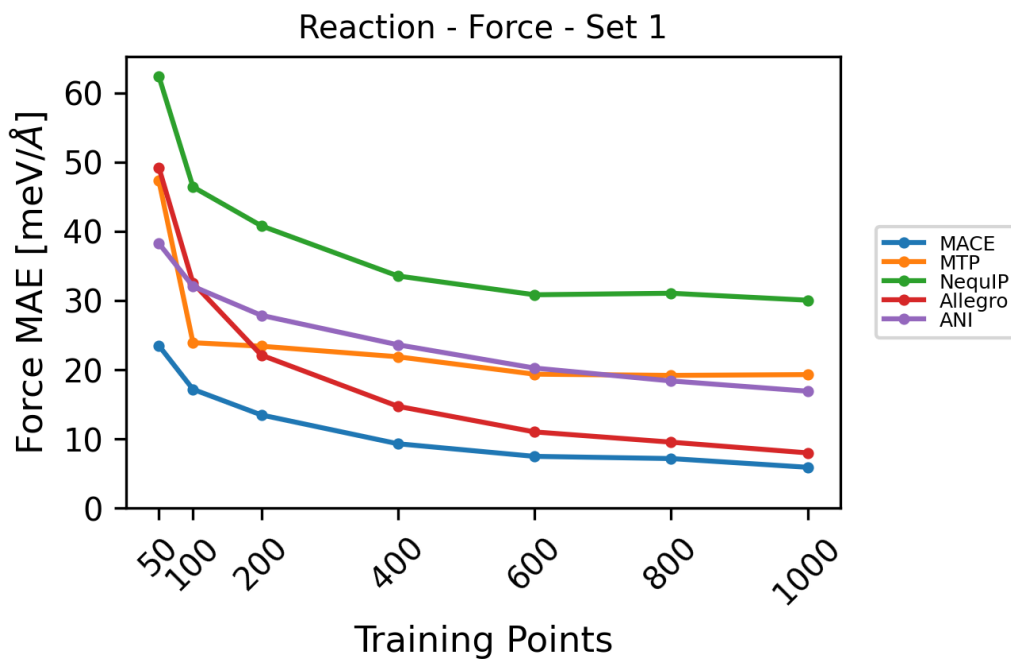**Figure S180.** Force mean absolute error vs training points for Reaction, Set 2. Unit: meV/Å.

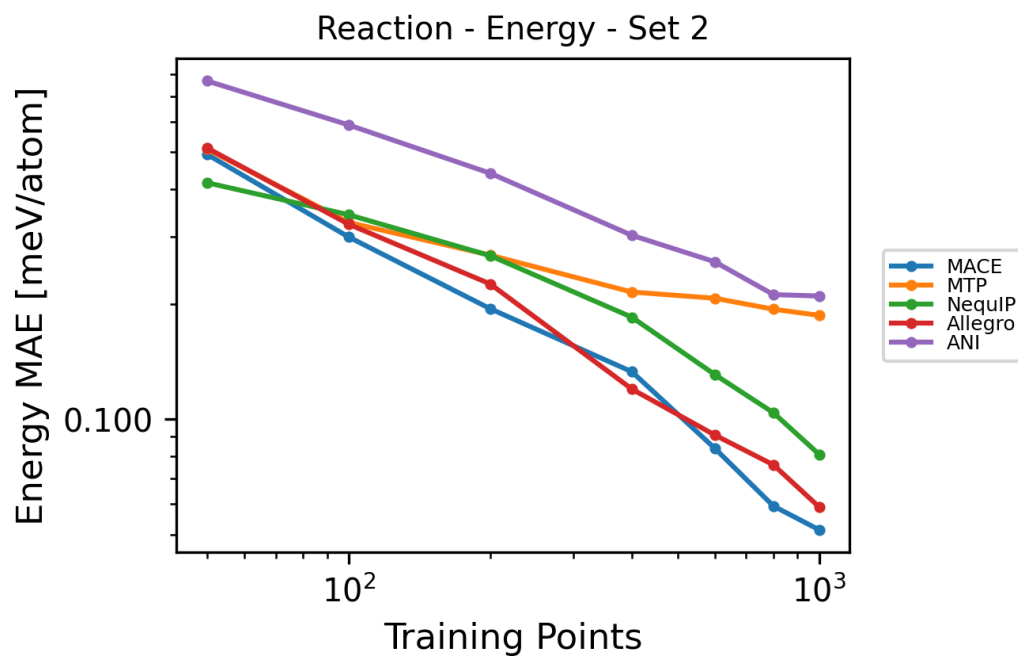**Figure S181.** Energy mean absolute error vs training points for Reaction, Set 3. Unit: meV/atom.

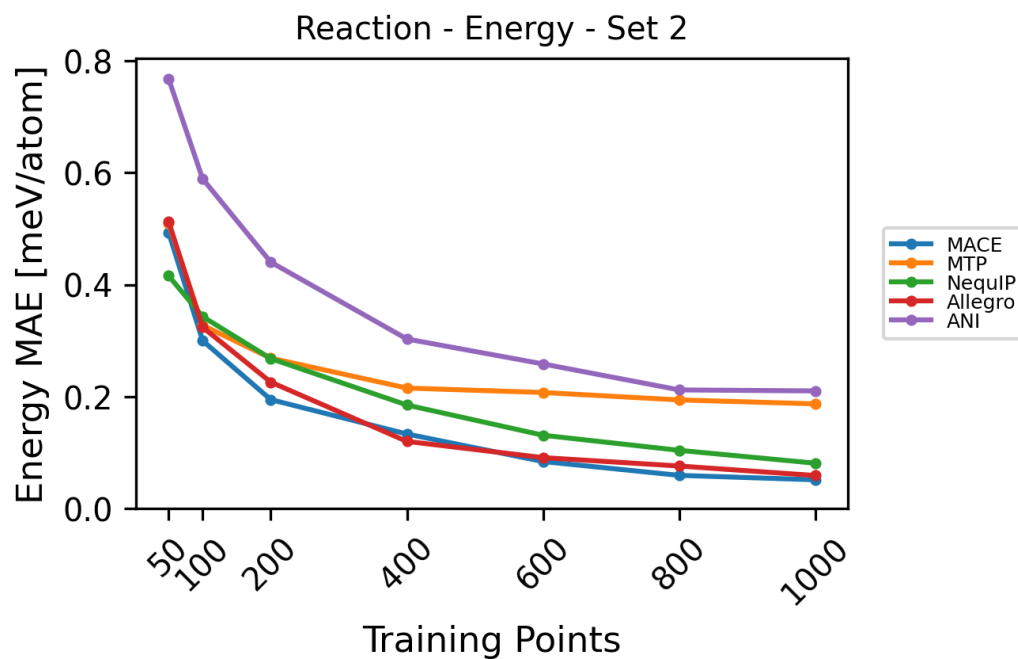**Figure S182.** Energy mean absolute error vs training points for Reaction, Set 3. Unit: meV/atom.

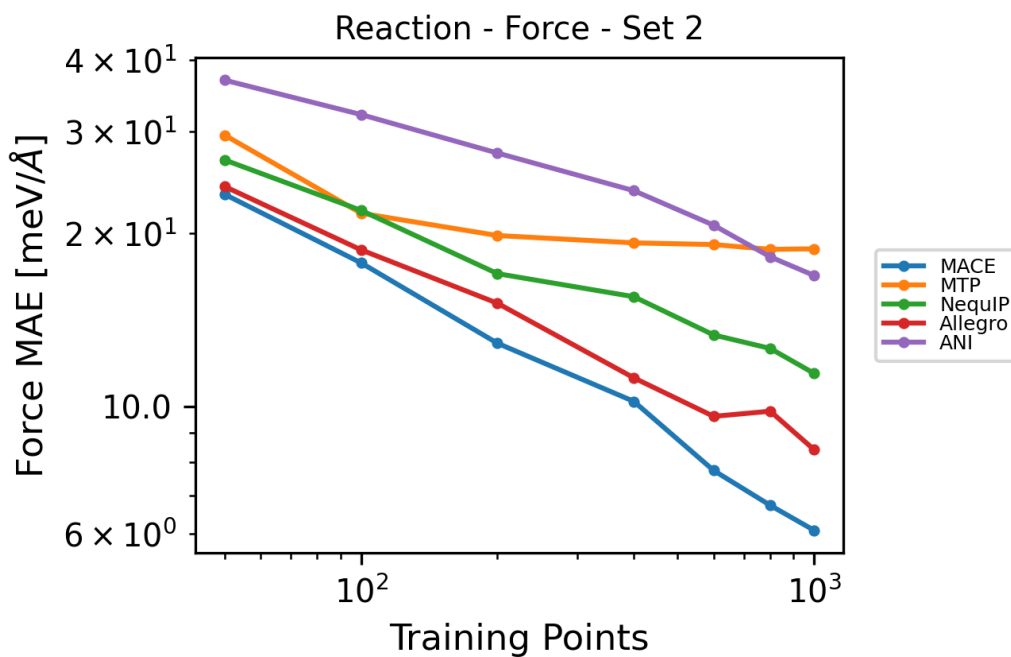**Figure S183.** Force mean absolute error vs training points for Reaction, Set 3. Unit: meV/Å.

Figure S184. Force mean absolute error vs training points for Reaction, Set 3. Unit: meV/Å.

Figure S185. Energy mean absolute error vs training points for Reaction, Set mean. Unit: meV/atom.
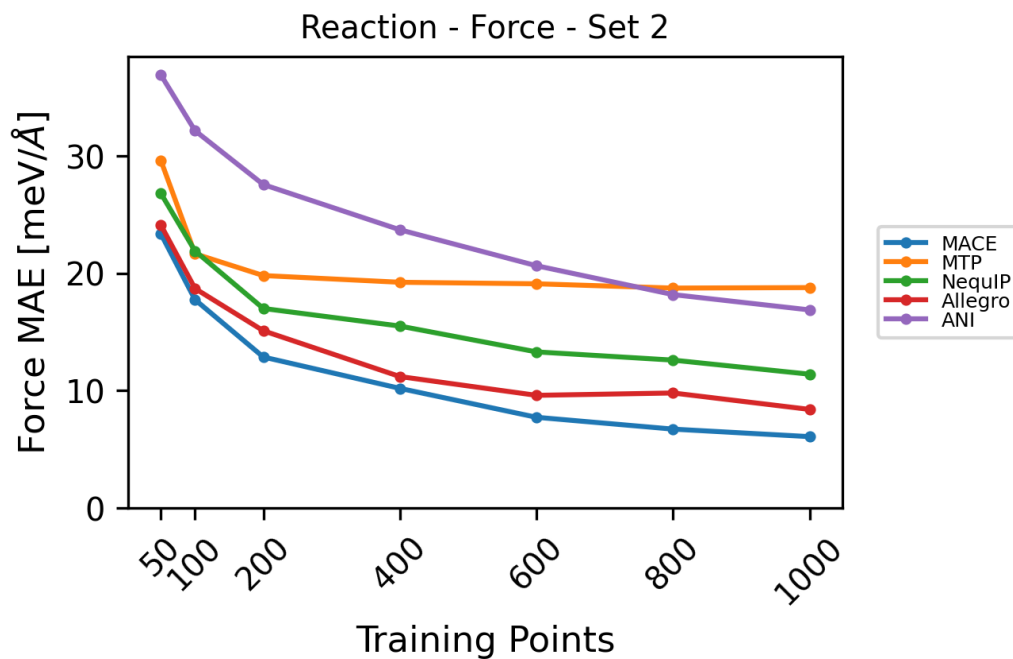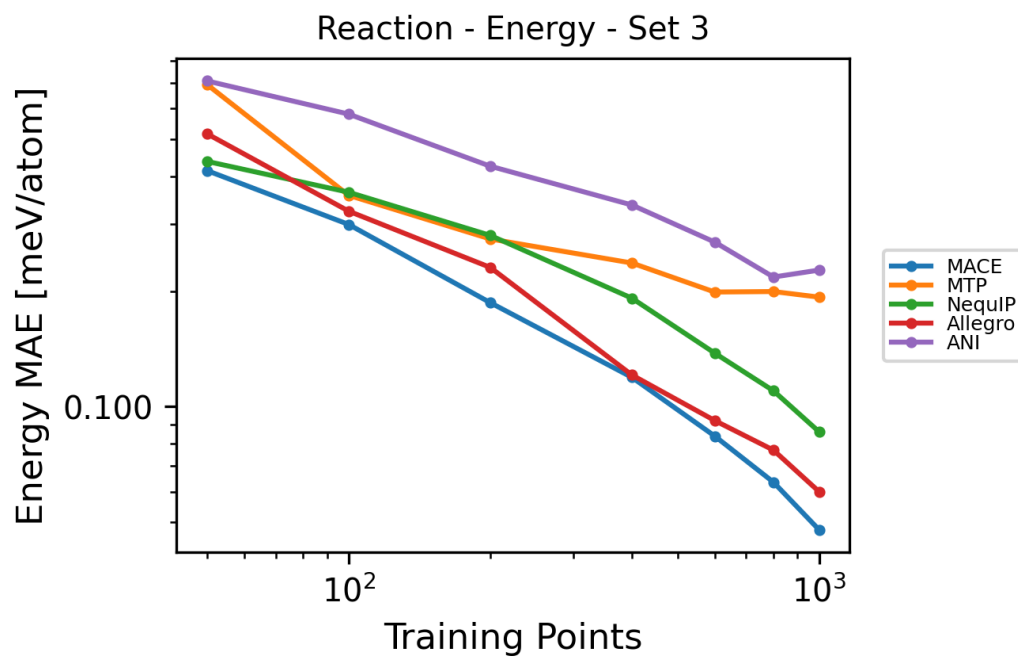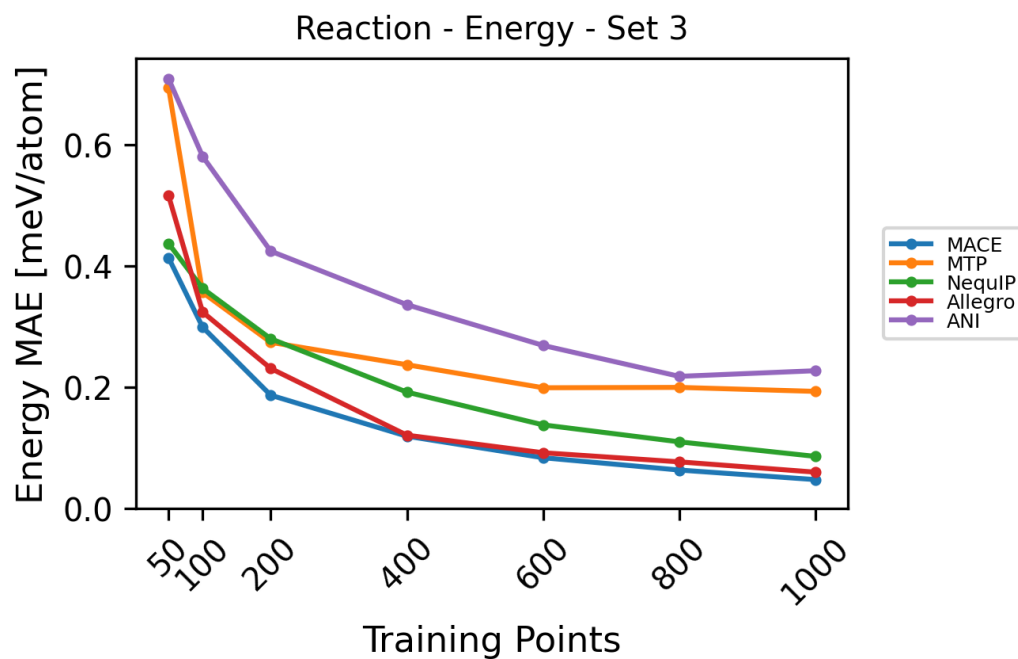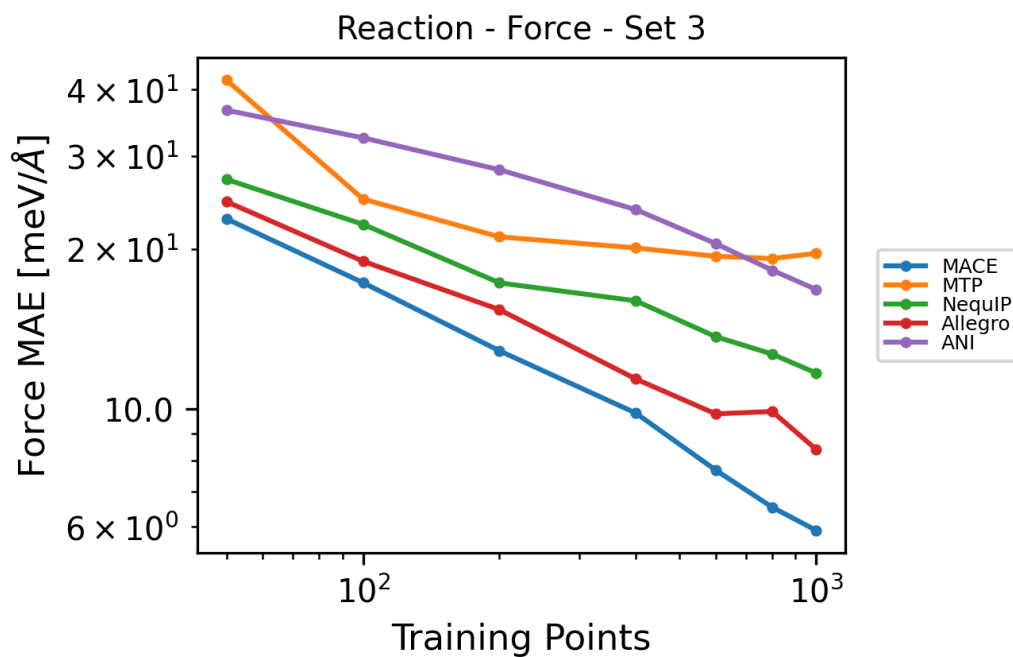
Figure S186. Energy mean absolute error vs training points for Reaction, Set mean. Unit: meV/atom.

Figure S187. Force mean absolute error vs training points for Reaction, Set mean. Unit: meV/Å.

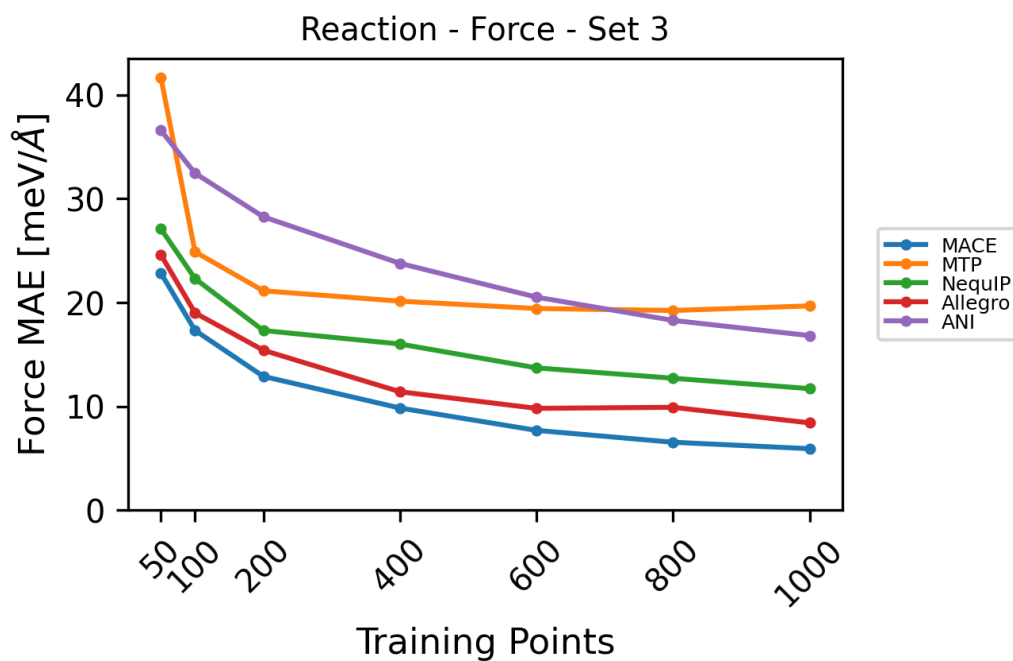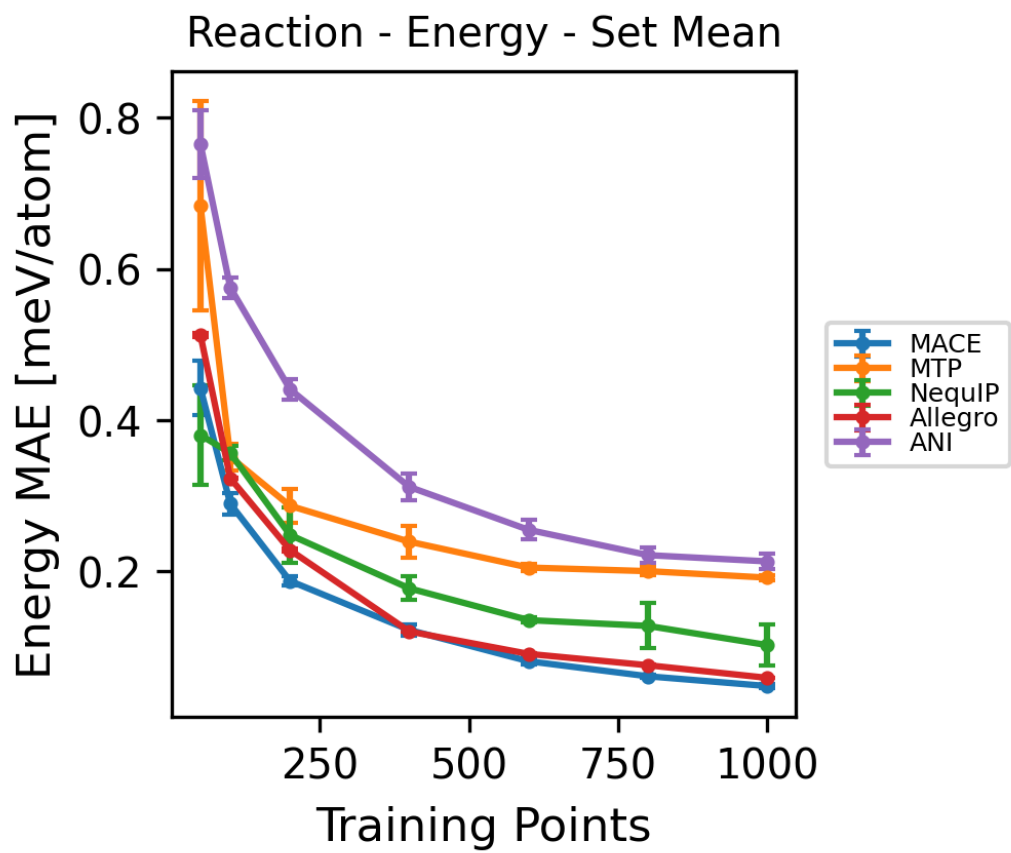**Figure S188.** Force mean absolute error vs training points for Reaction, Set mean. Unit: meV/Å.

HEA

Figure S189. Energy mean absolute error vs training points for HEA, Set 1. Unit: meV/atom.

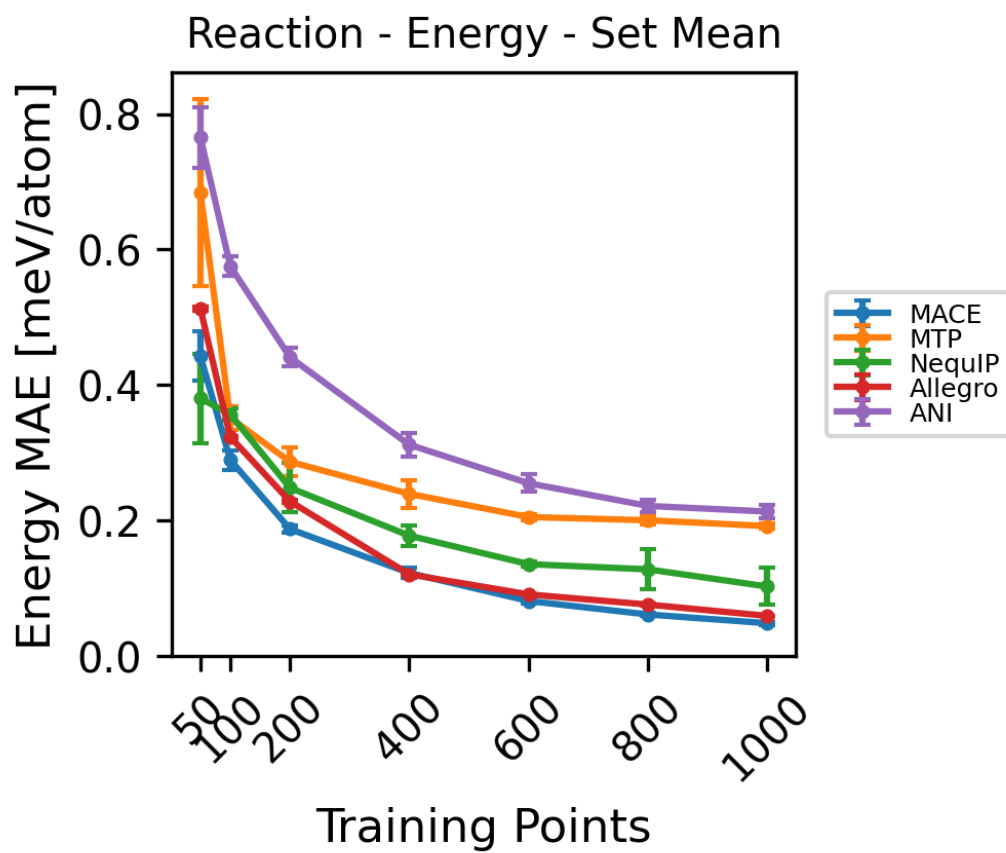**Figure S190.** Energy mean absolute error vs training points for HEA, Set 1. Unit: meV/atom.

Figure S191. Force mean absolute error vs training points for HEA, Set 1. Unit: meV/Å.

Figure S192. Force mean absolute error vs training points for HEA, Set 1. Unit: meV/Å.

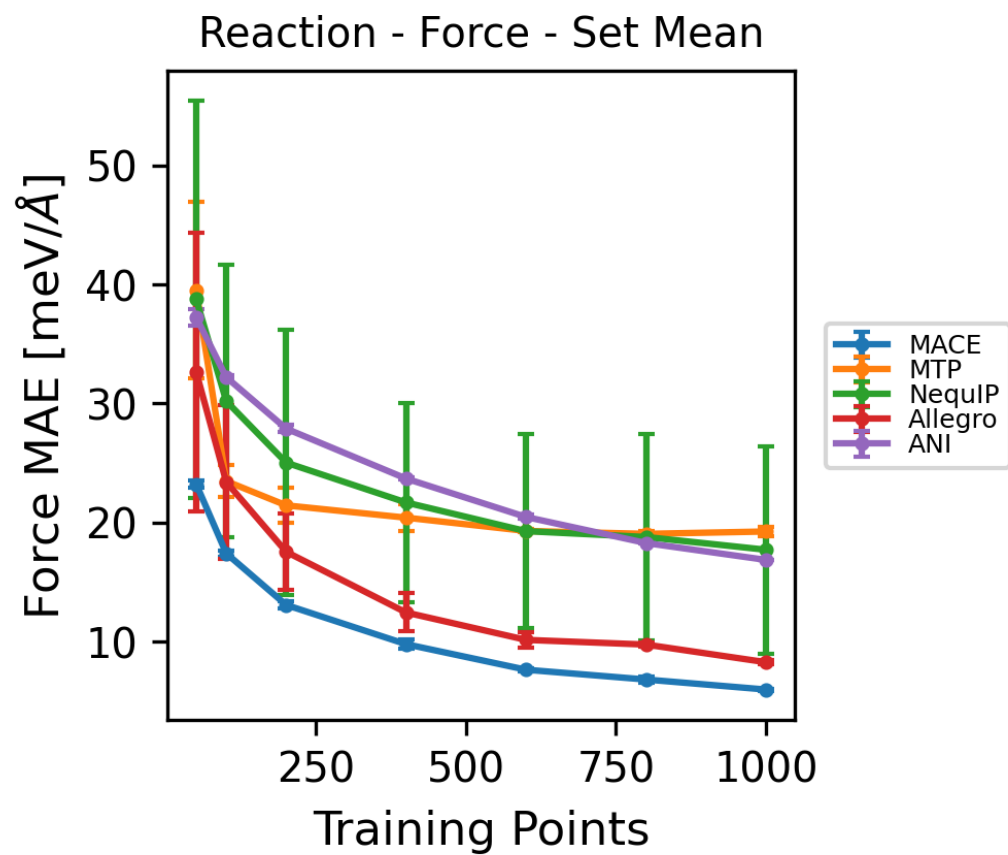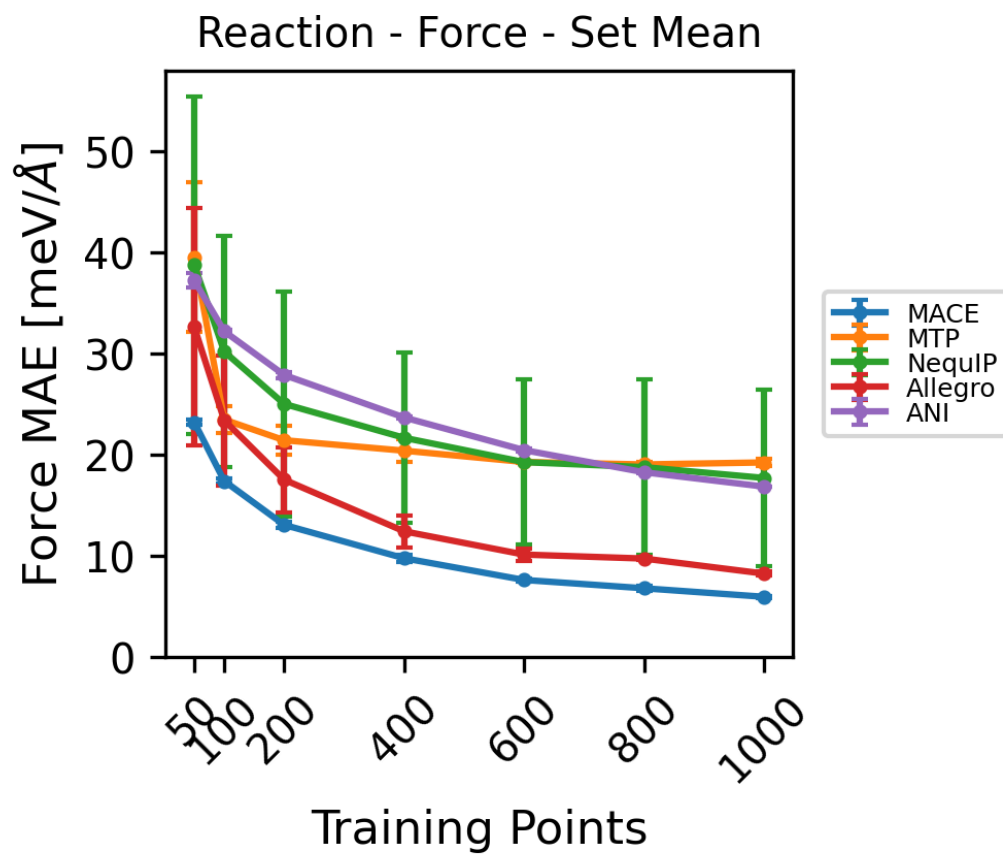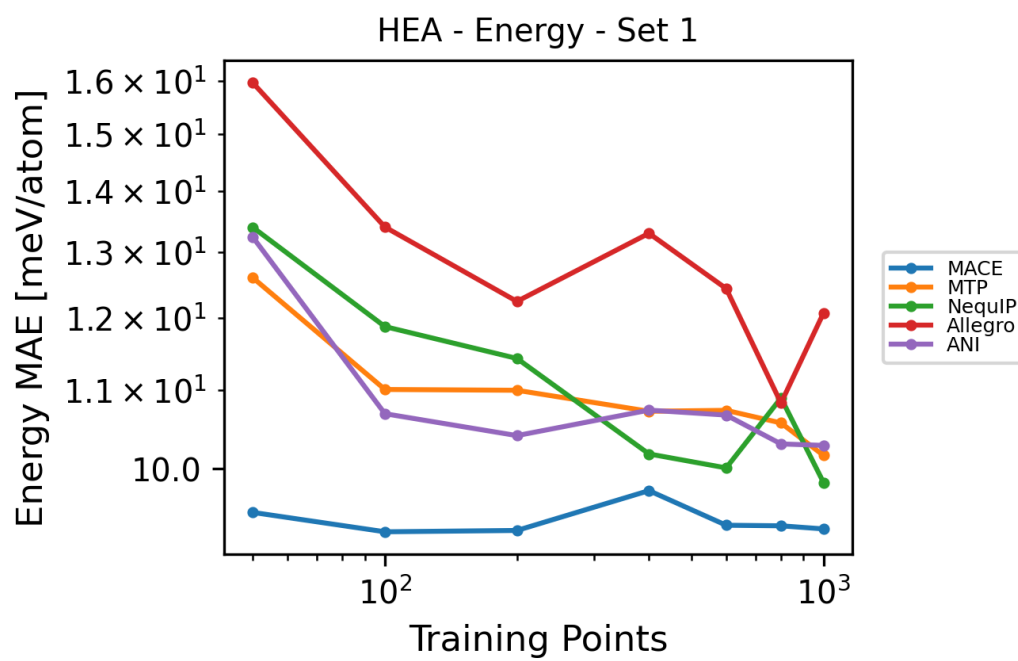**Figure S193.** Stress mean absolute error vs training points for HEA, Set 1. Unit: meV/Å².

Figure S194. Stress mean absolute error vs training points for HEA, Set 1. Unit: meV/Å².

Figure S195. Energy mean absolute error vs training points for HEA, Set 2. Unit: meV/atom.

Figure S196. Energy mean absolute error vs training points for HEA, Set 2. Unit: meV/atom.

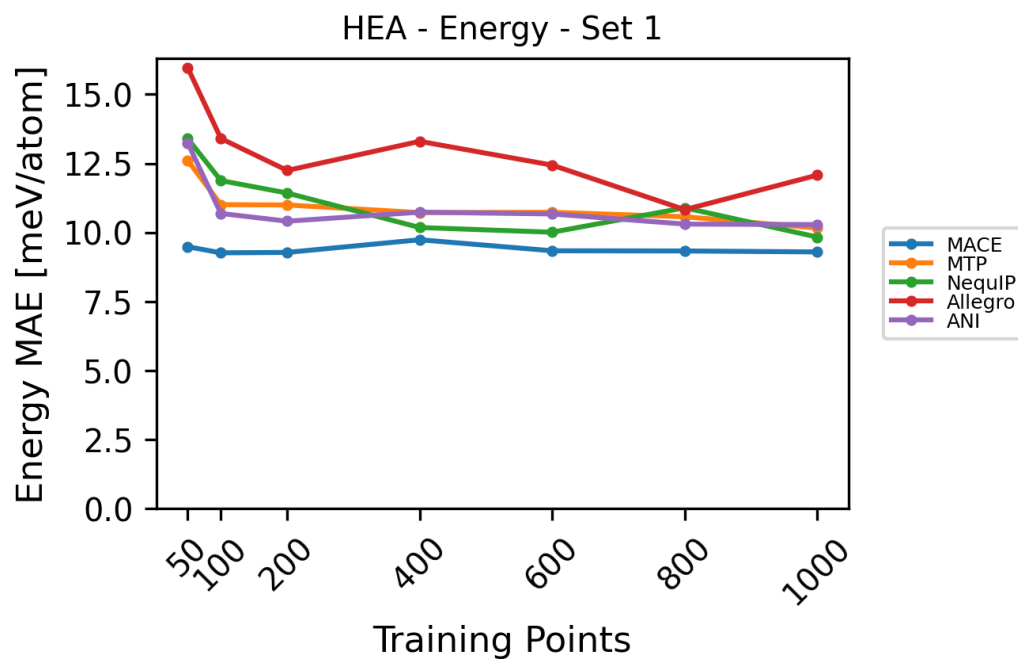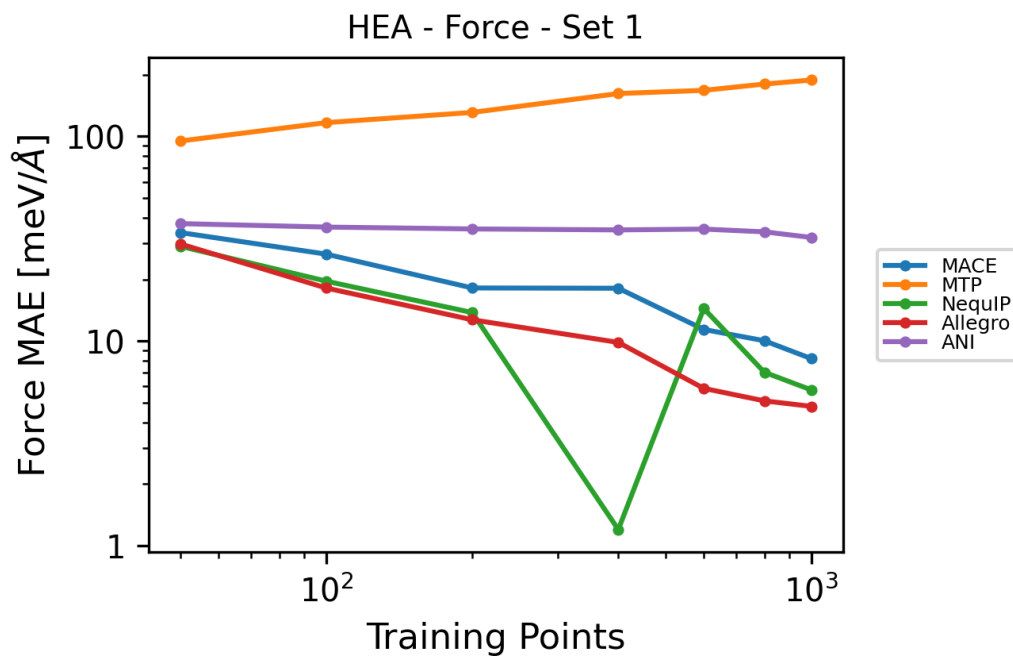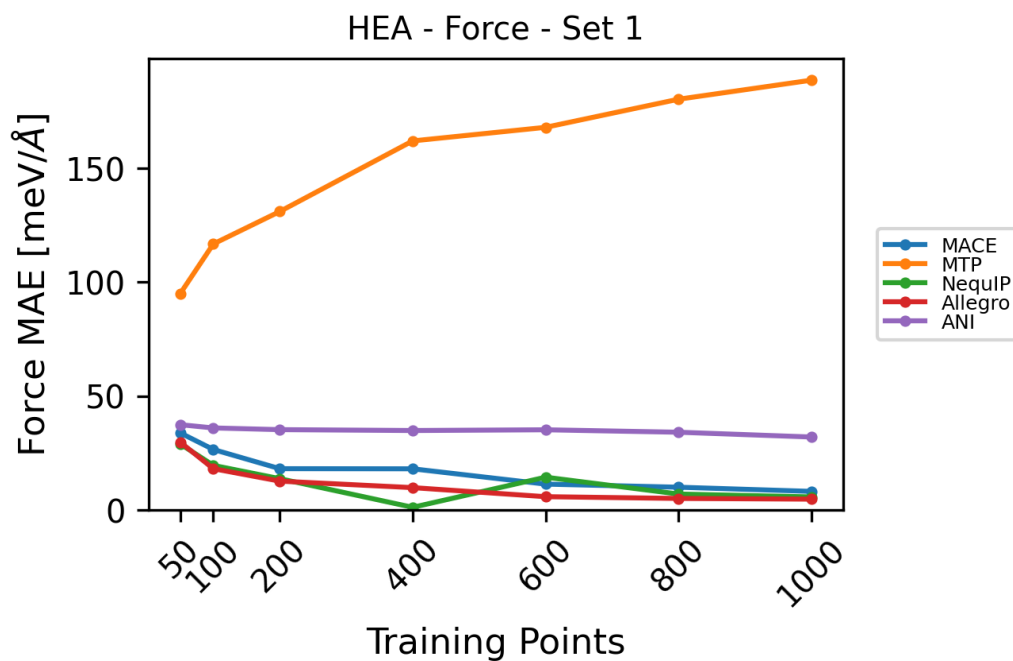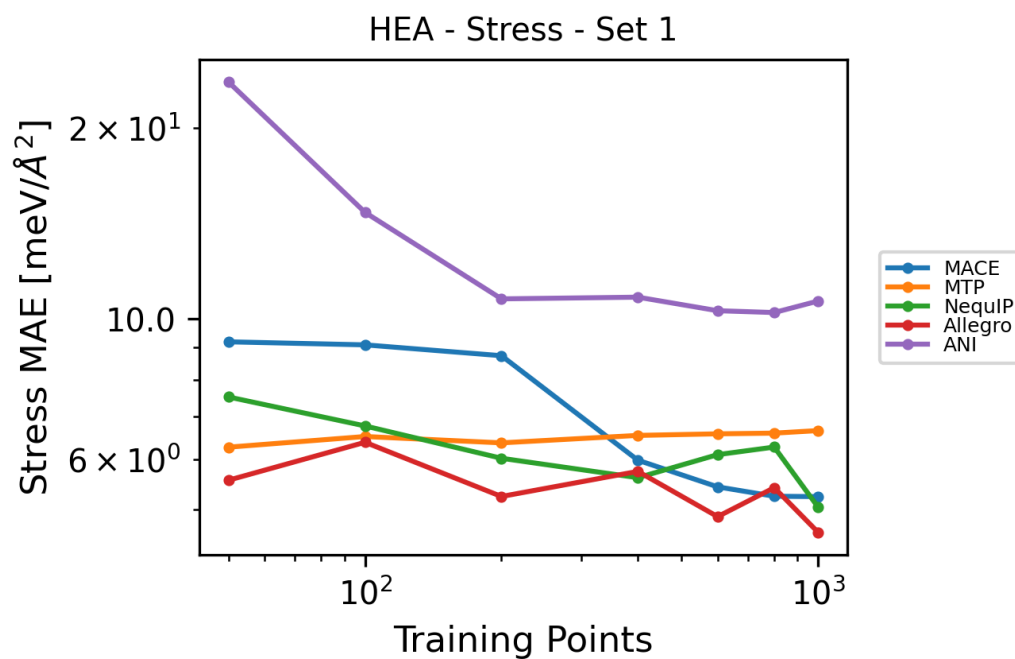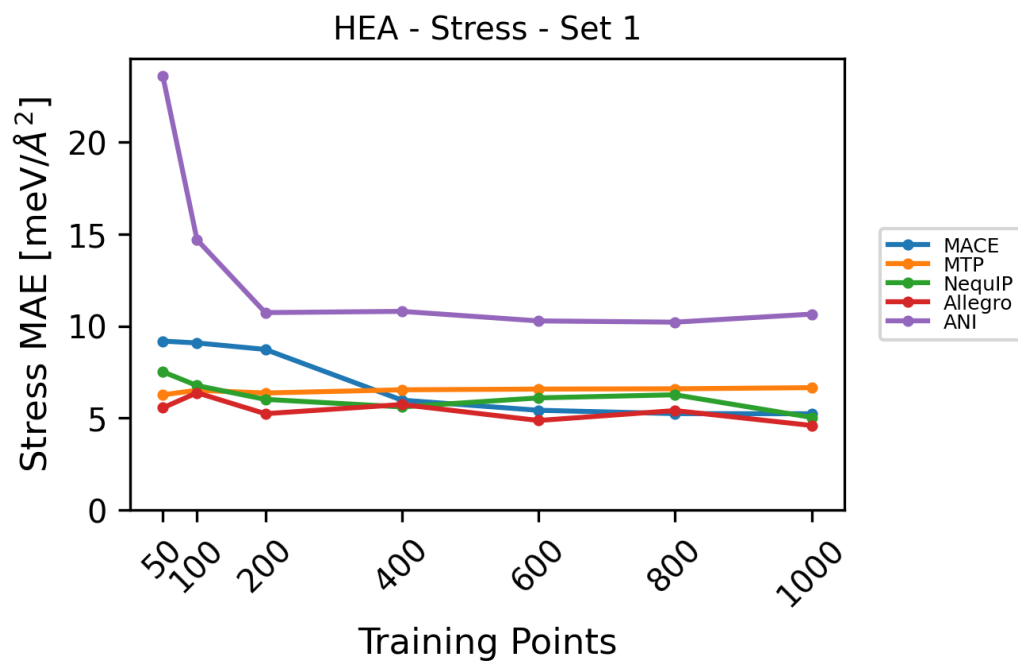**Figure S197.** Force mean absolute error vs training points for HEA, Set 2. Unit: meV/Å.
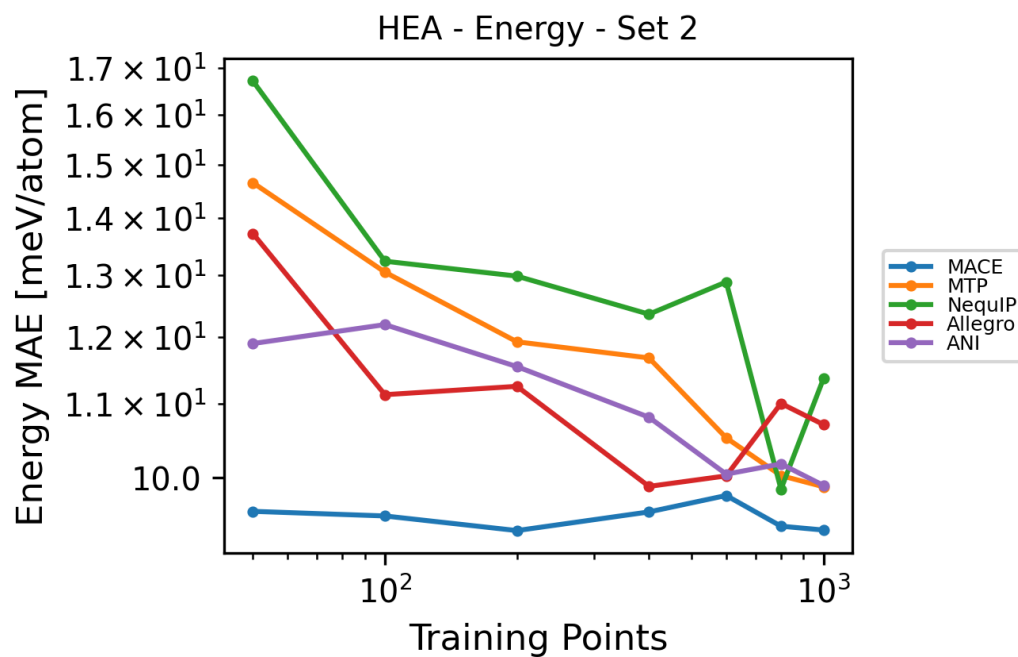
Figure S198. Force mean absolute error vs training points for HEA, Set 2. Unit: meV/Å.

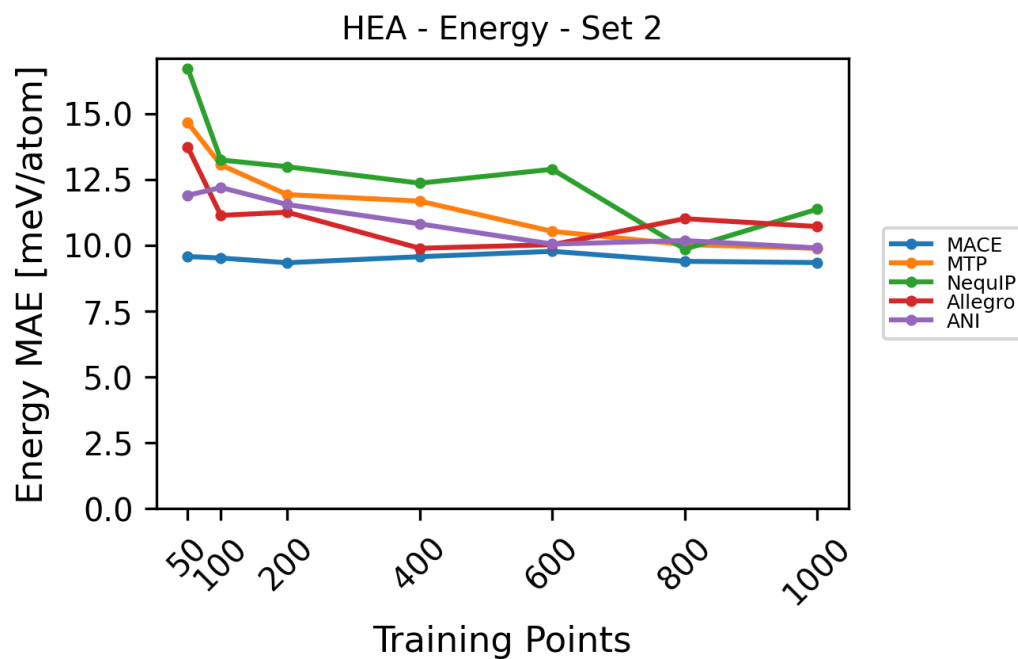**Figure S199.** Stress mean absolute error vs training points for HEA, Set 2. Unit: meV/Å².

Figure S200. Stress mean absolute error vs training points for HEA, Set 2. Unit: meV/Å².
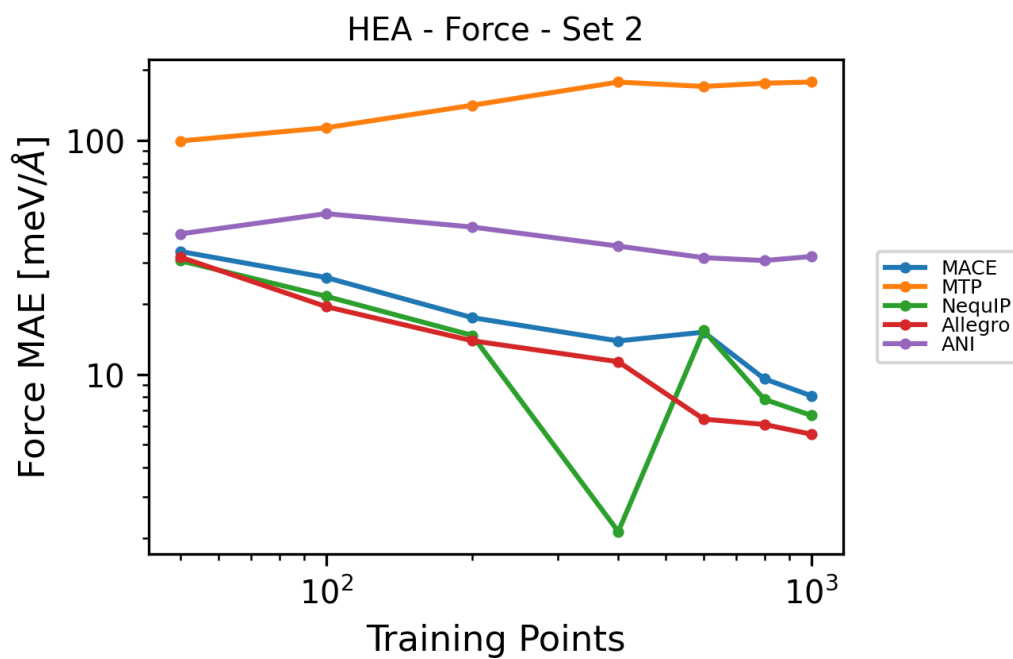
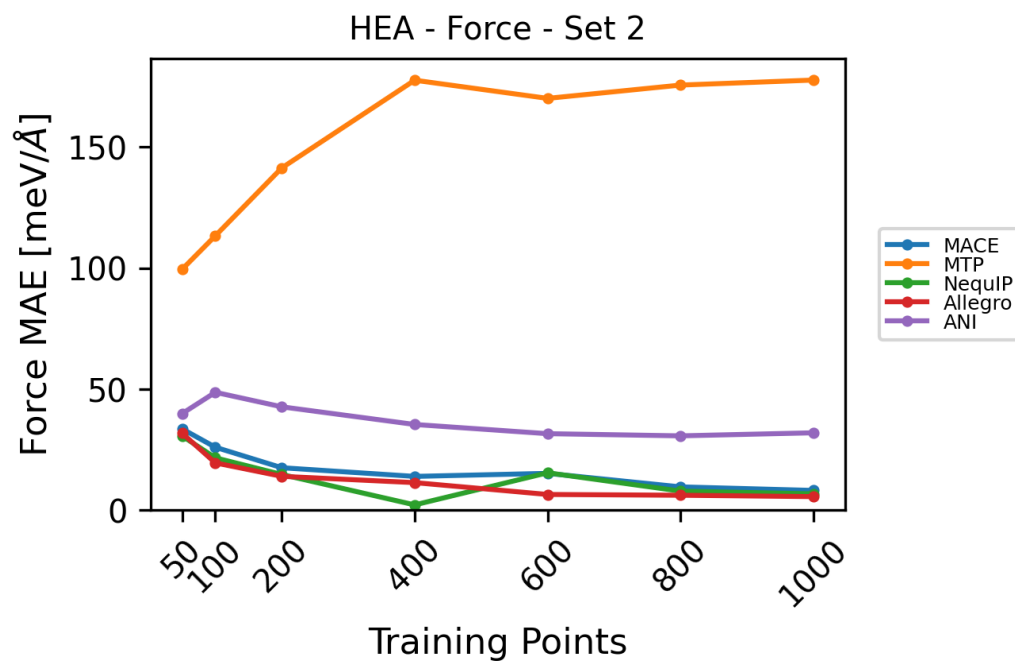**Figure S201.** Energy mean absolute error vs training points for HEA, Set 3. Unit: meV/atom.
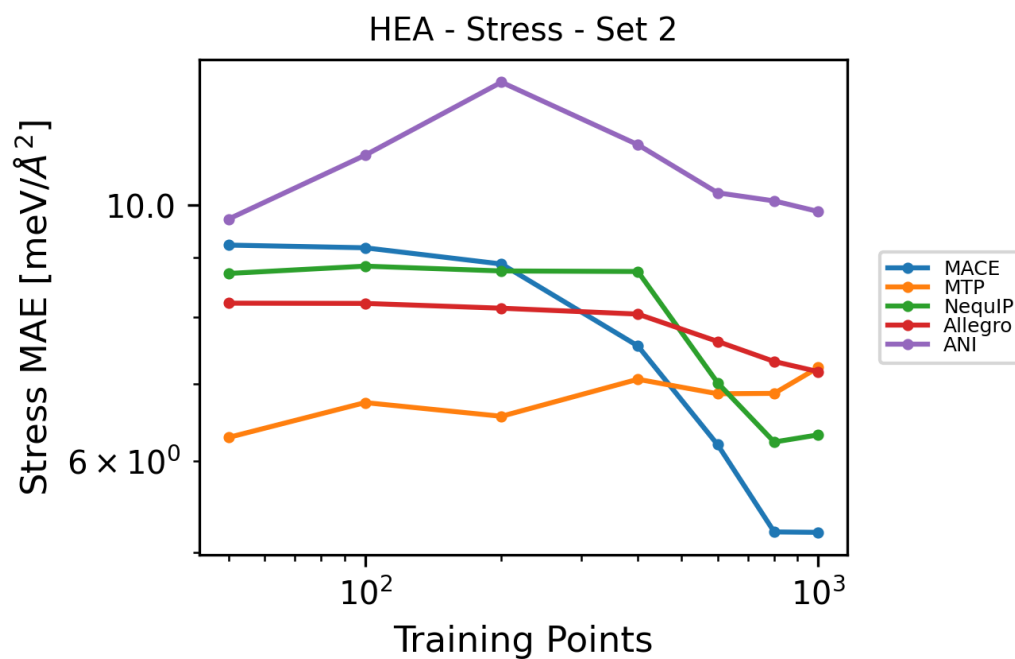
Figure S202. Energy mean absolute error vs training points for HEA, Set 3. Unit: meV/atom.
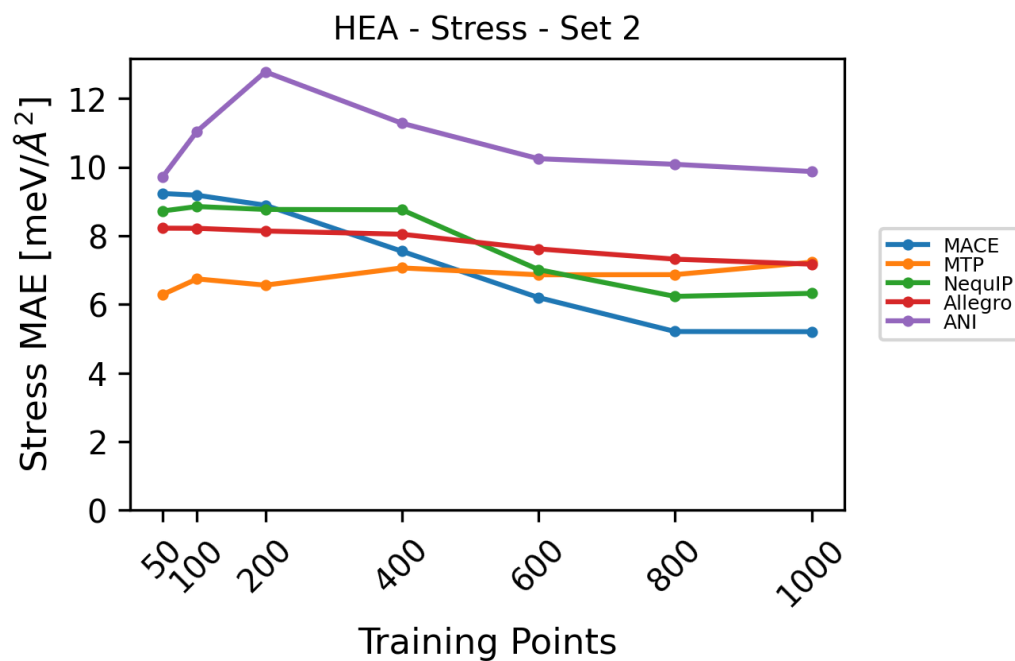
Figure S203. Force mean absolute error vs training points for HEA, Set 3. Unit: meV/Å.
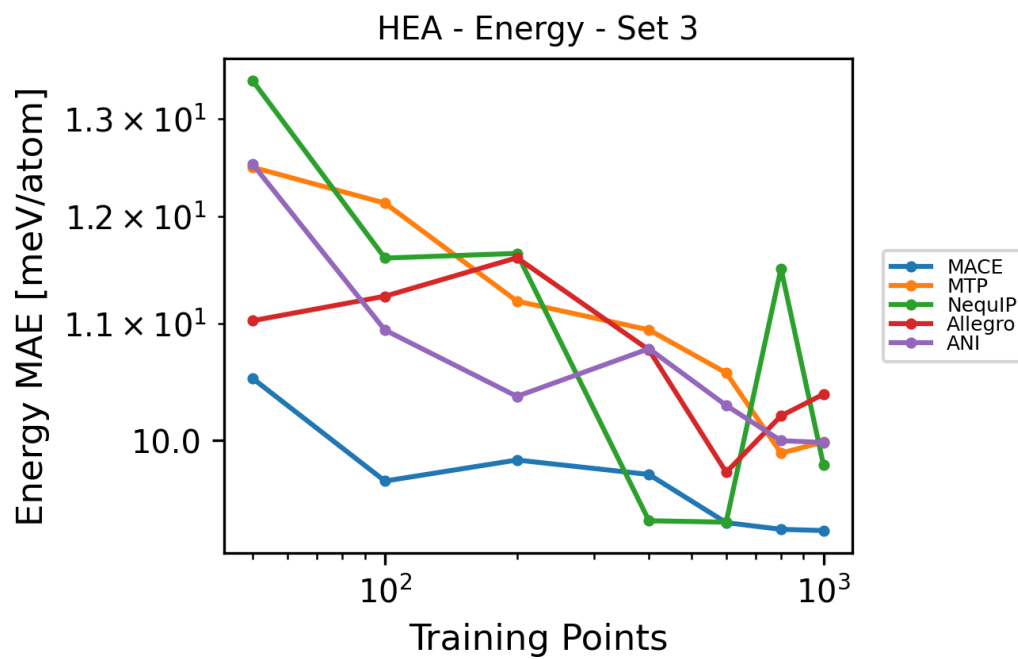
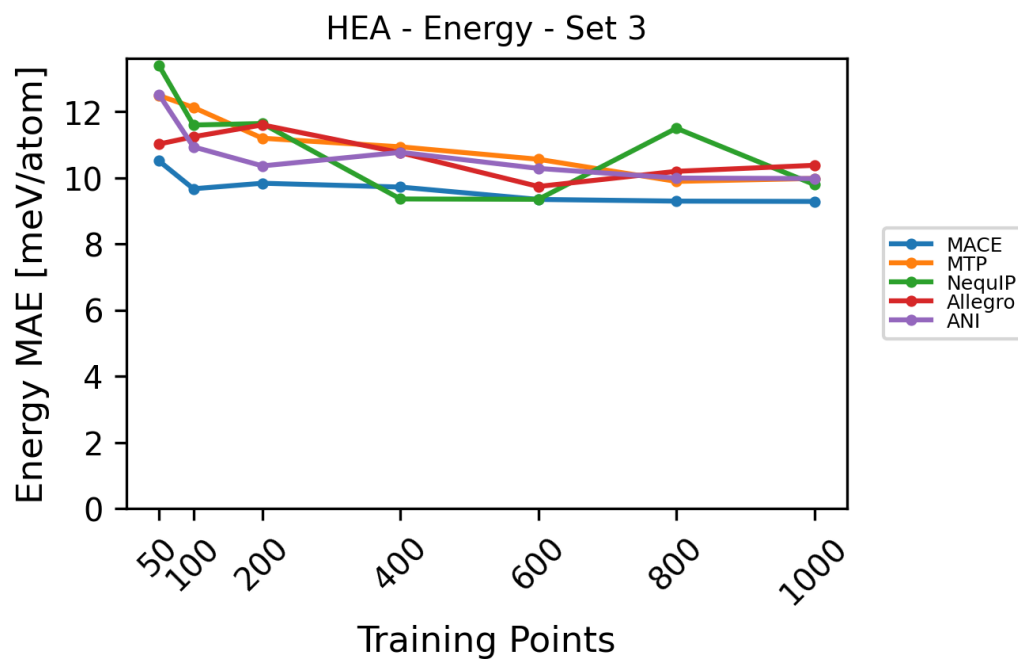**Figure S204.** Force mean absolute error vs training points for HEA, Set 3. Unit: meV/Å.

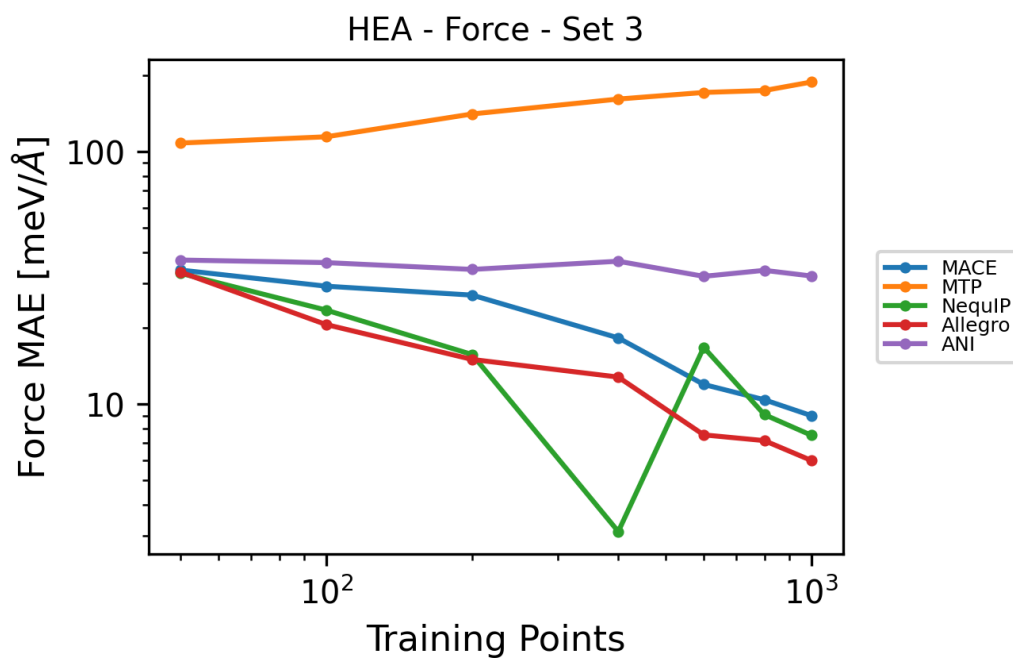**Figure S205.** Stress mean absolute error vs training points for HEA, Set 3. Unit: meV/Å².

Figure S206. Stress mean absolute error vs training points for HEA, Set 3. Unit: meV/Å².

Figure S207. Energy mean absolute error vs training points for HEA, Set mean. Unit: meV/atom.
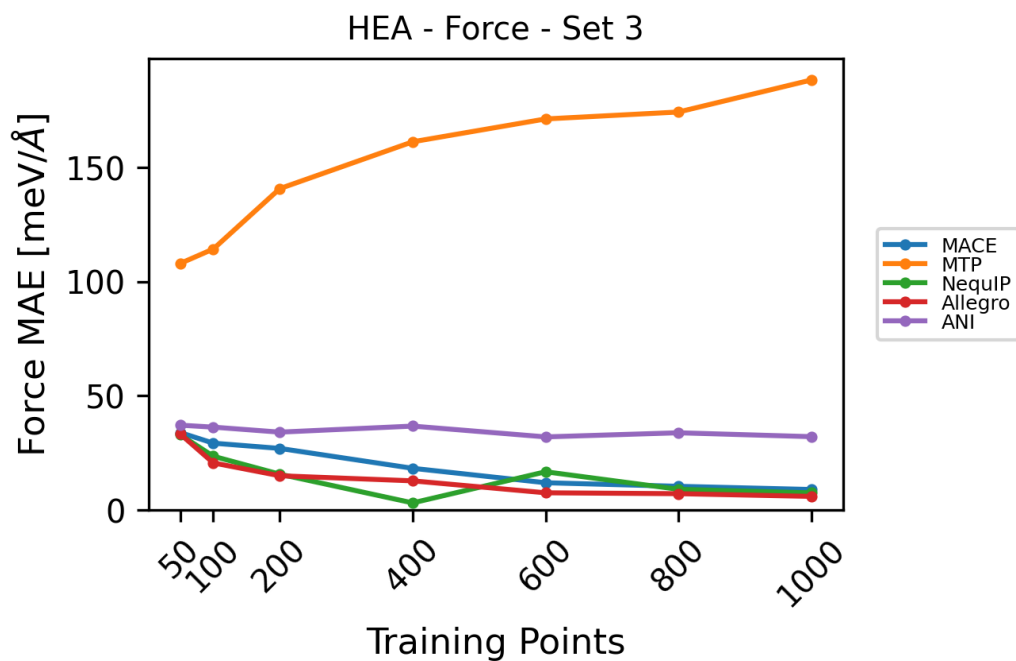
Figure S208. Energy mean absolute error vs training points for HEA, Set mean. Unit: meV/atom.
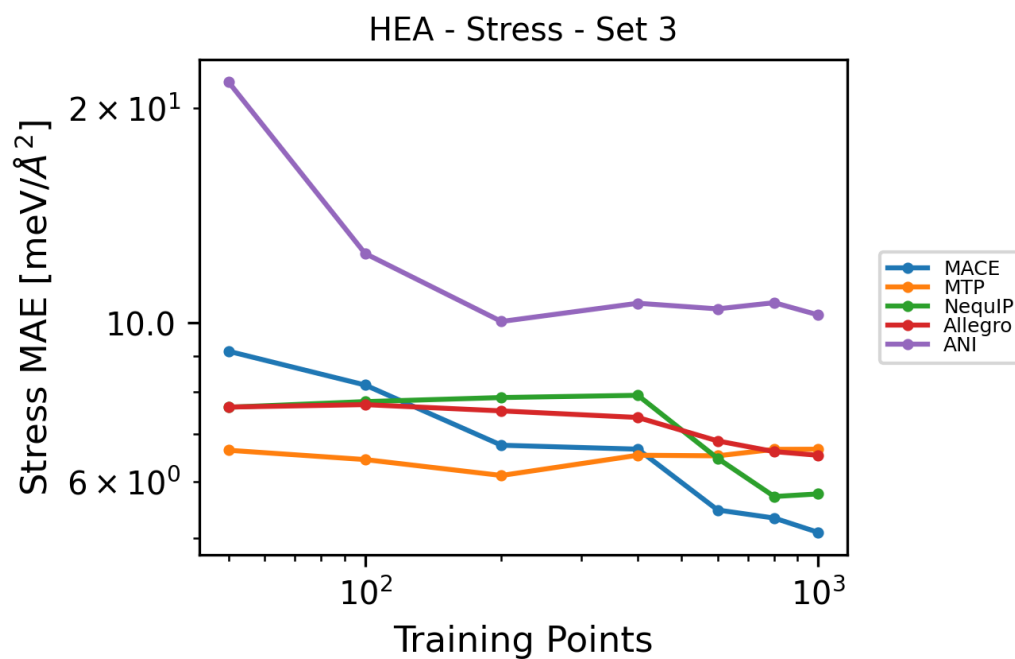
Figure S209. Force mean absolute error vs training points for HEA, Set mean. Unit: meV/Å.
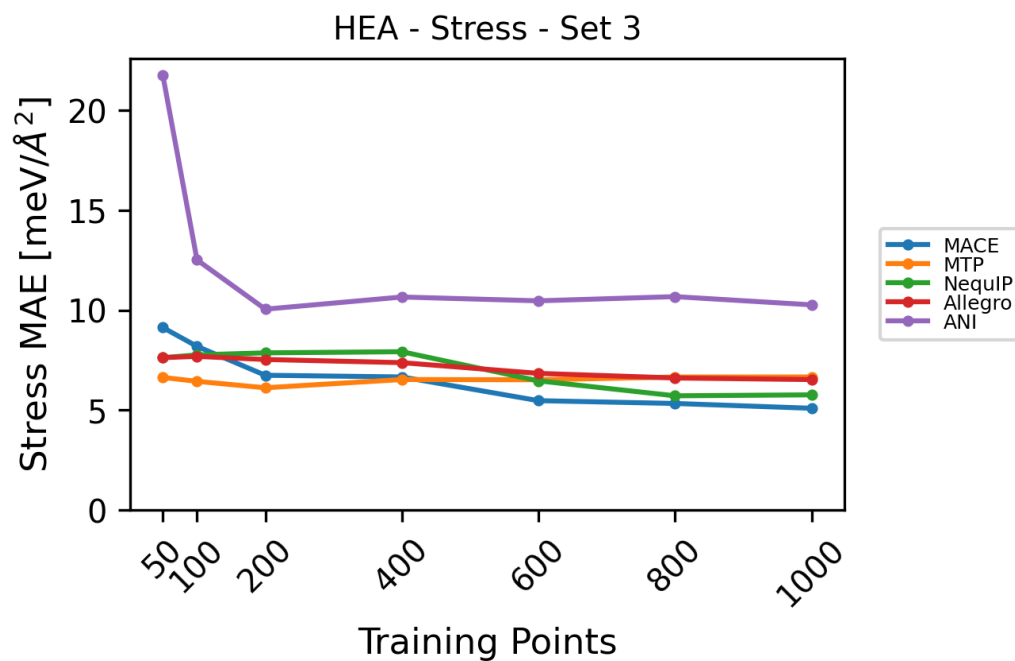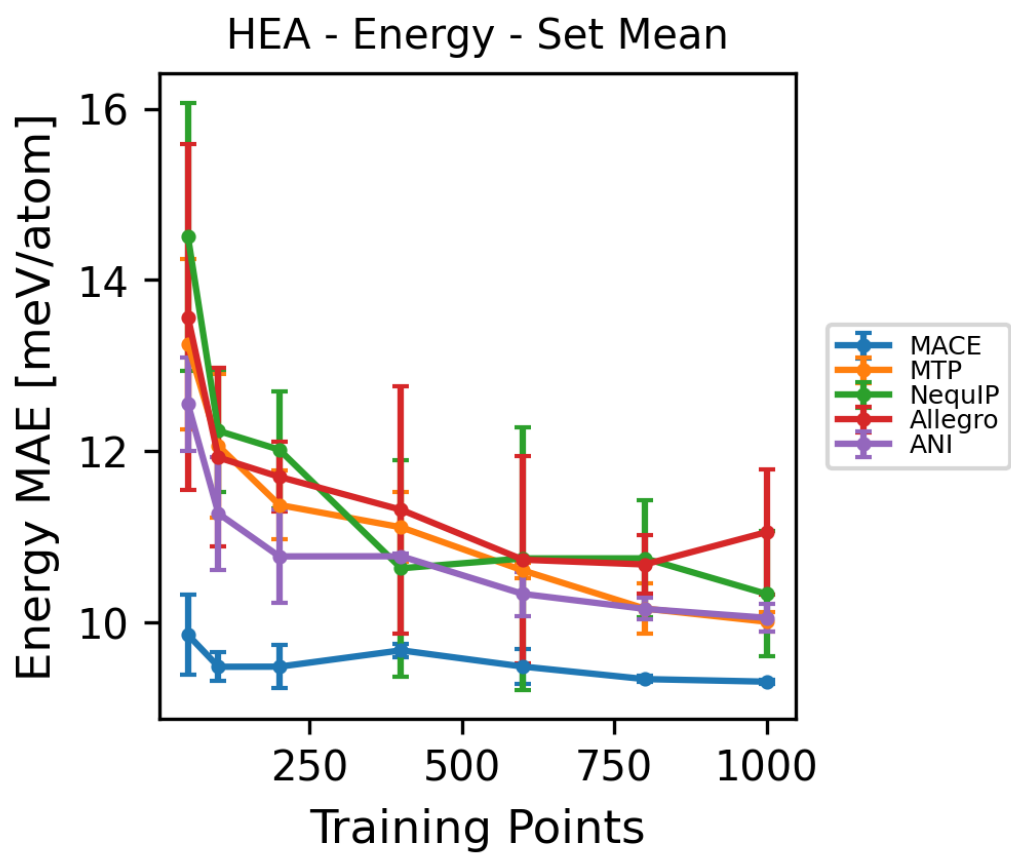
Figure S210. Force mean absolute error vs training points for HEA, Set mean. Unit: meV/Å.
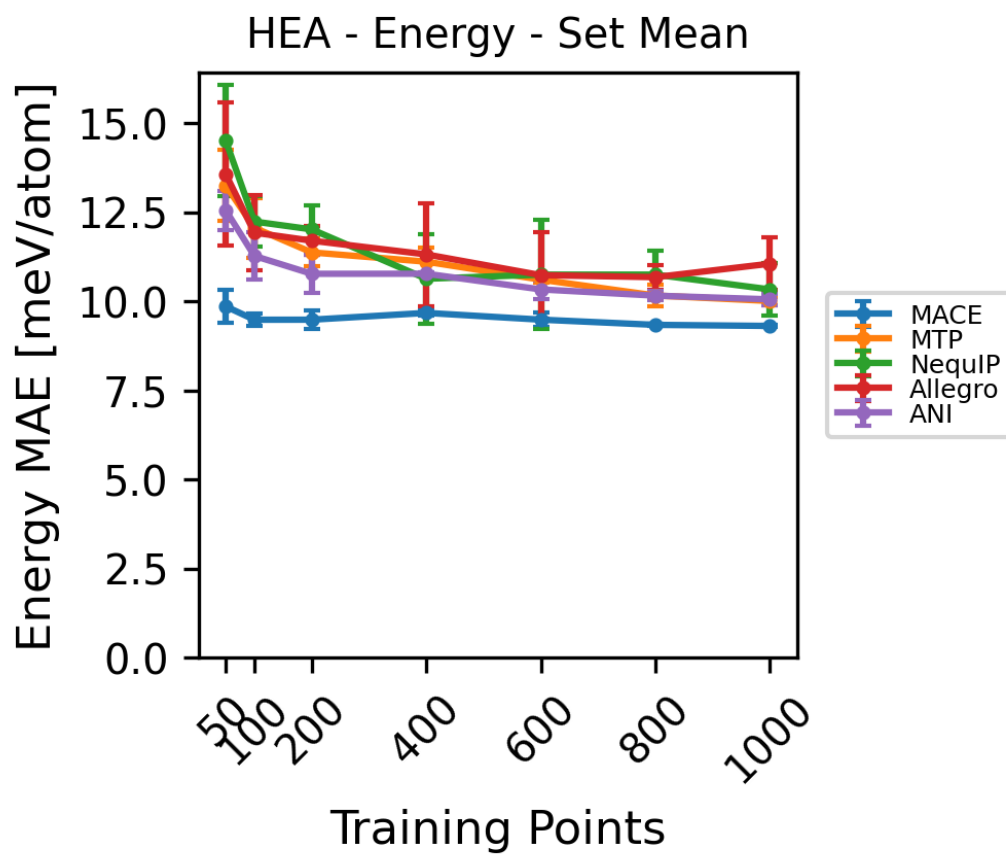
Figure S211. Stress mean absolute error vs training points for HEA, Set mean. Unit: meV/Å².

Figure S212. Stress mean absolute error vs training points for HEA, Set mean. Unit: meV/Å².

Zr-O

Figure S213. Energy mean absolute error vs training points for Zr-O, Set 1. Unit: meV/atom.

Figure S214. Energy mean absolute error vs training points for Zr-O, Set 1. Unit: meV/atom.

Figure S215. Force mean absolute error vs training points for Zr-O, Set 1. Unit: meV/Å.

Figure S216. Force mean absolute error vs training points for Zr-O, Set 1. Unit: meV/Å.

Figure S217. Stress mean absolute error vs training points for Zr-O, Set 1. Unit: meV/Å².
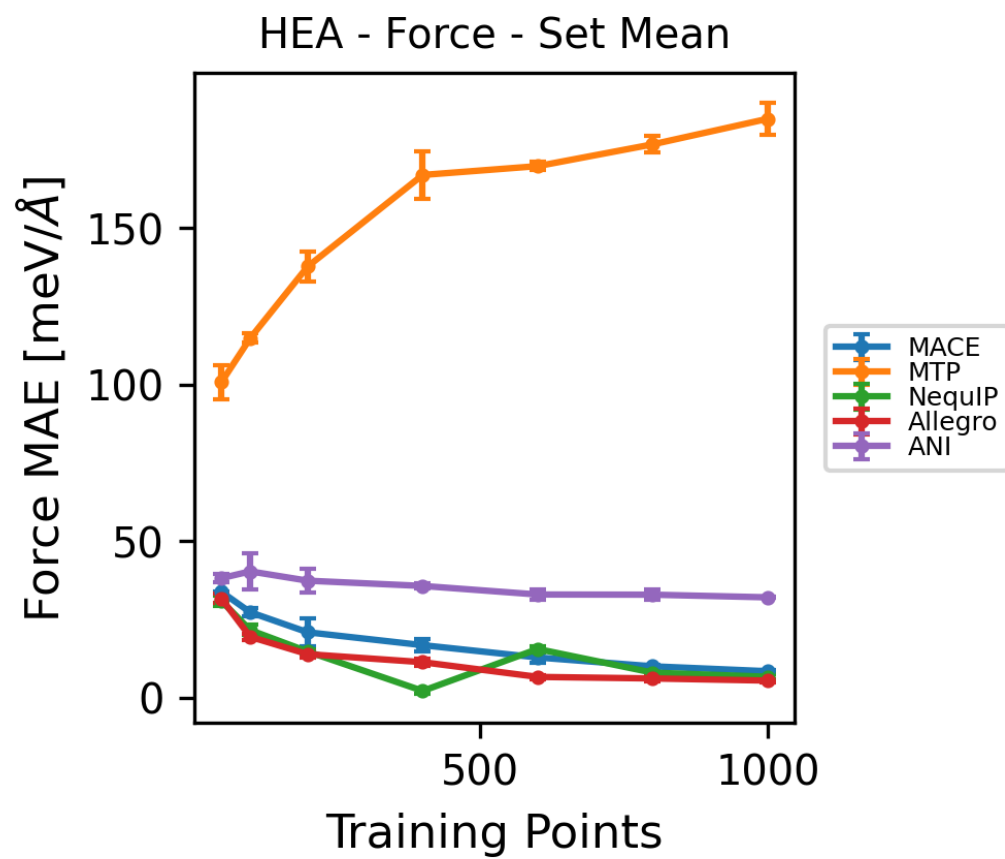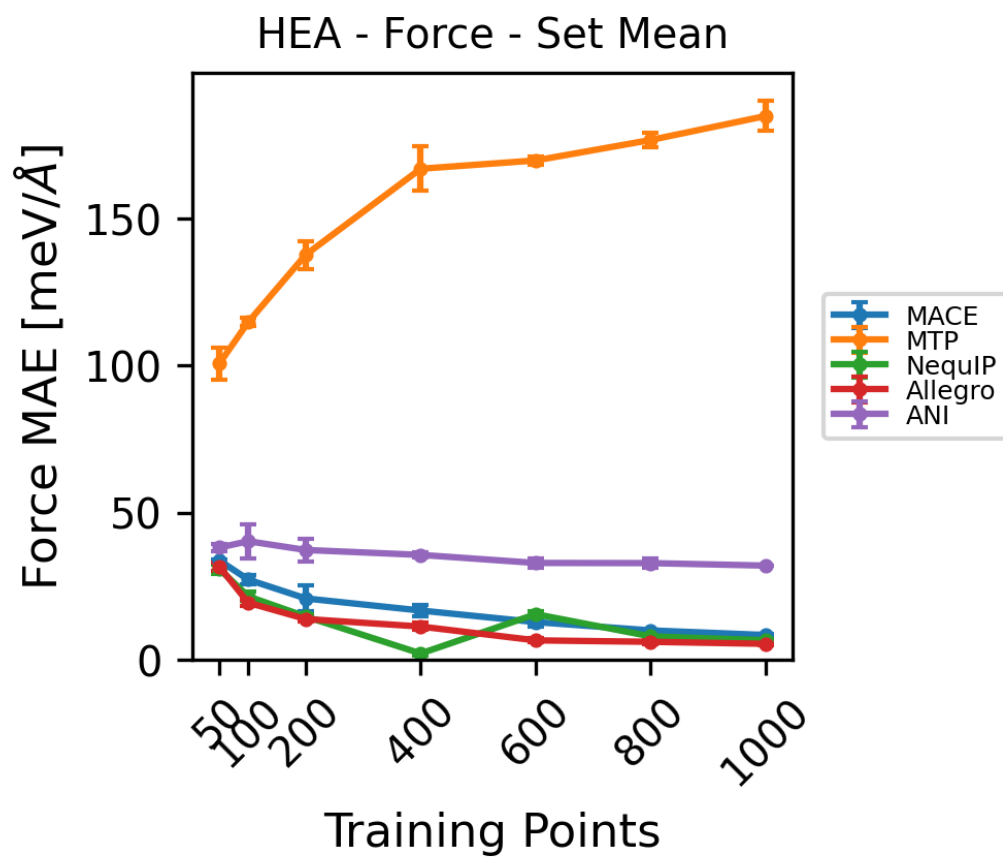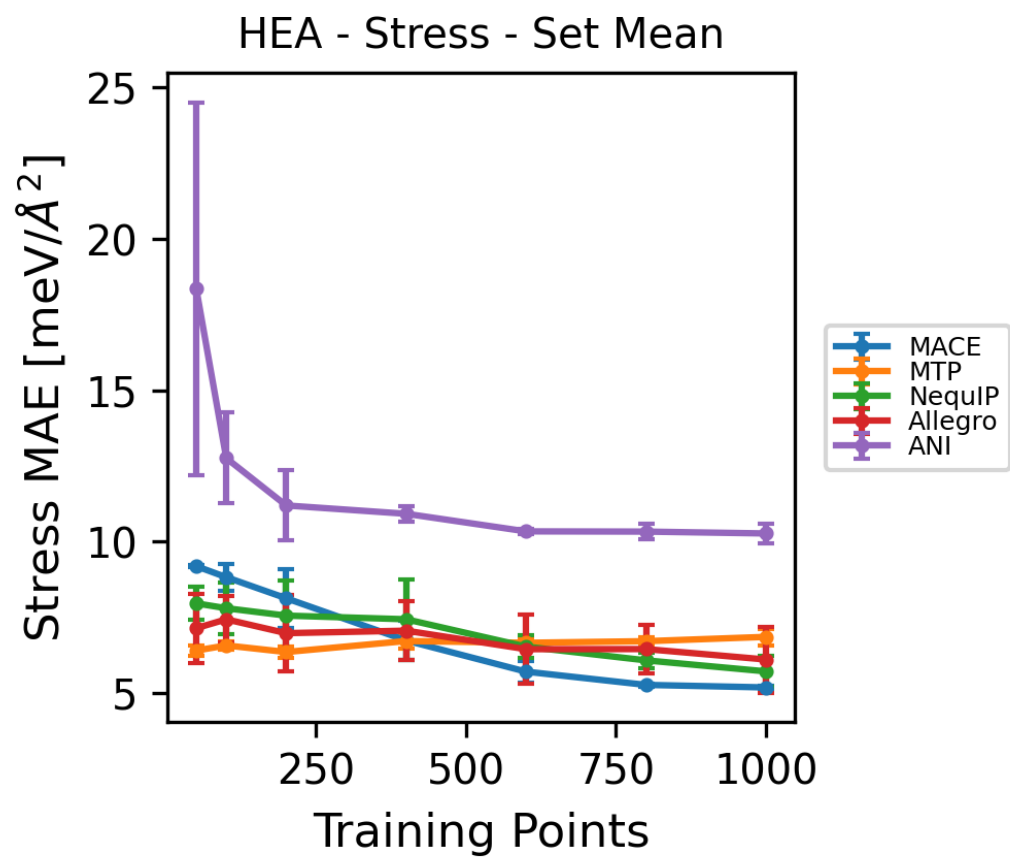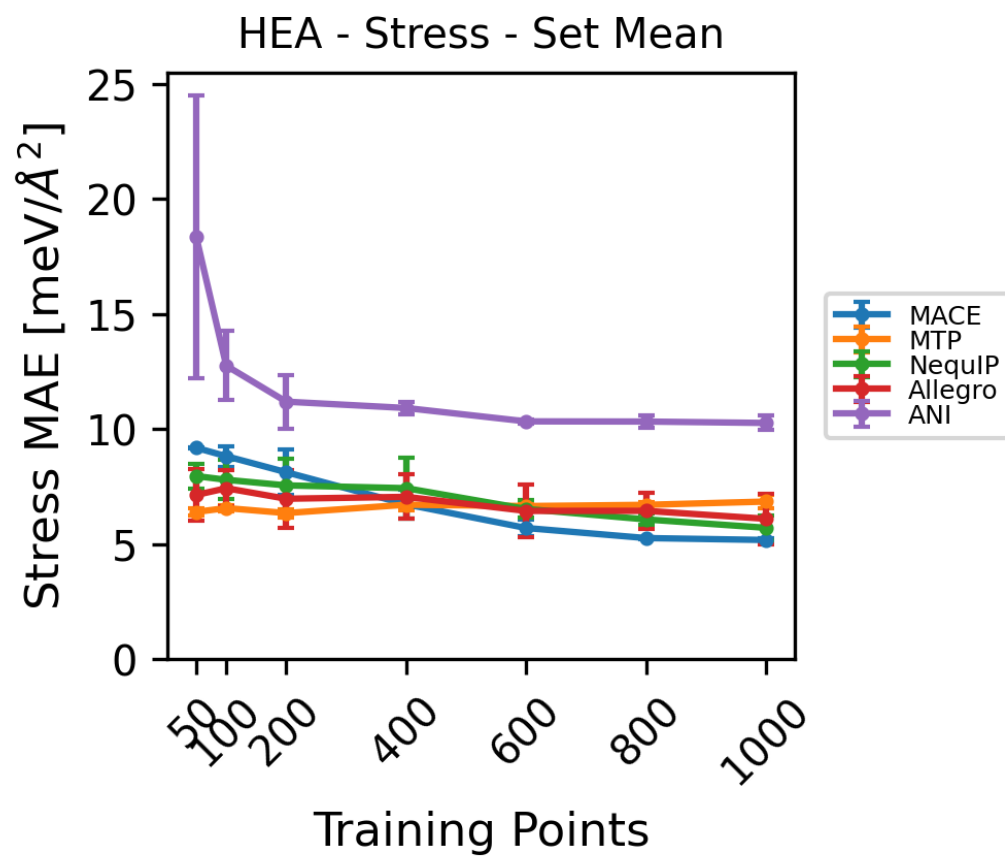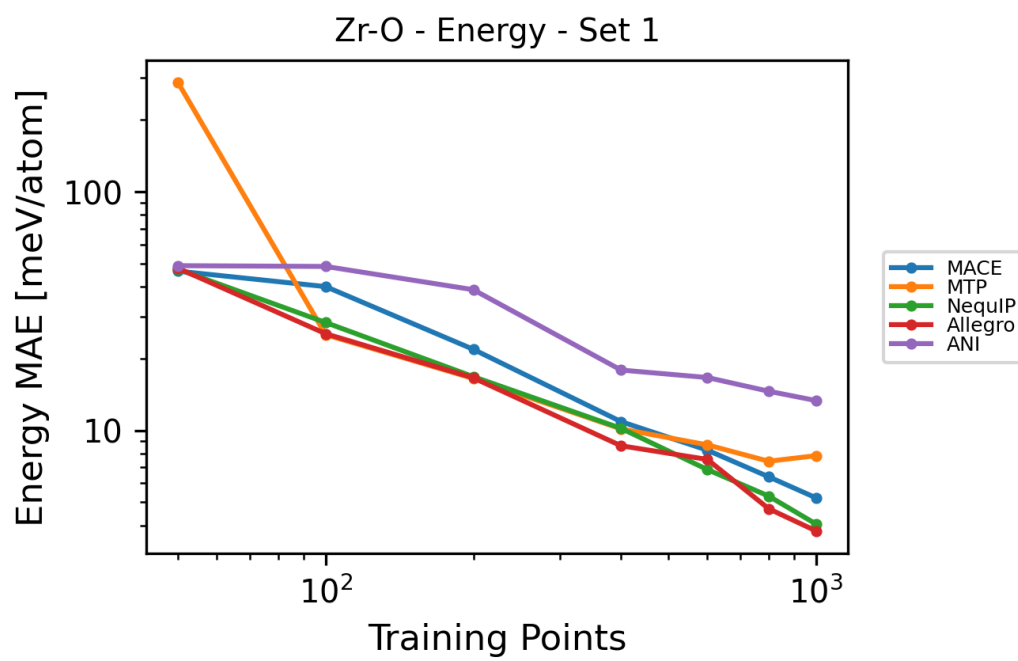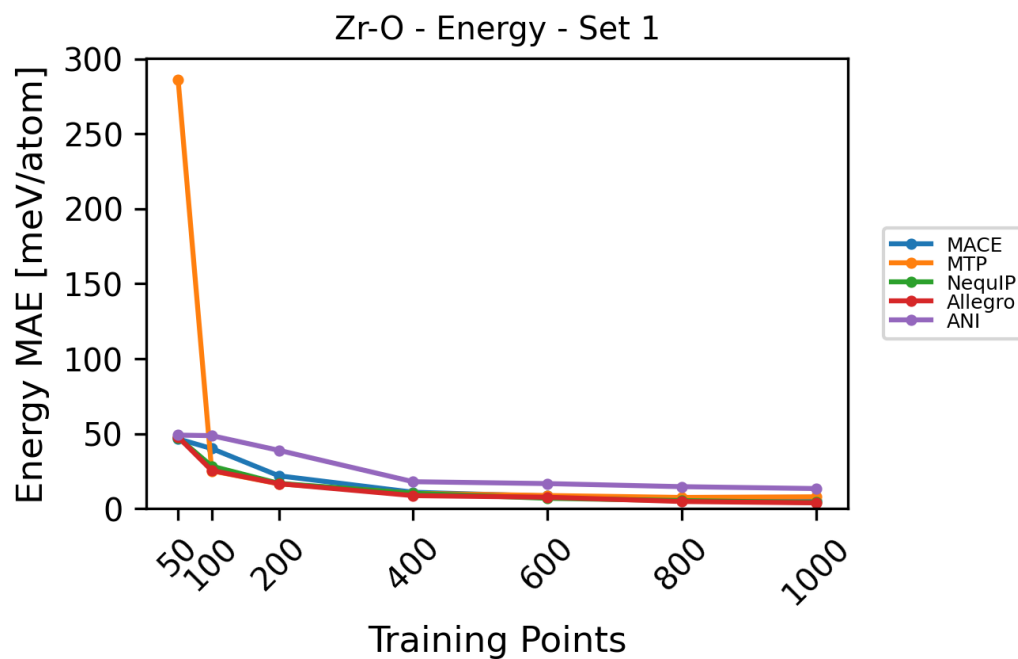
Figure S218. Stress mean absolute error vs training points for Zr-O, Set 1. Unit: meV/Å².
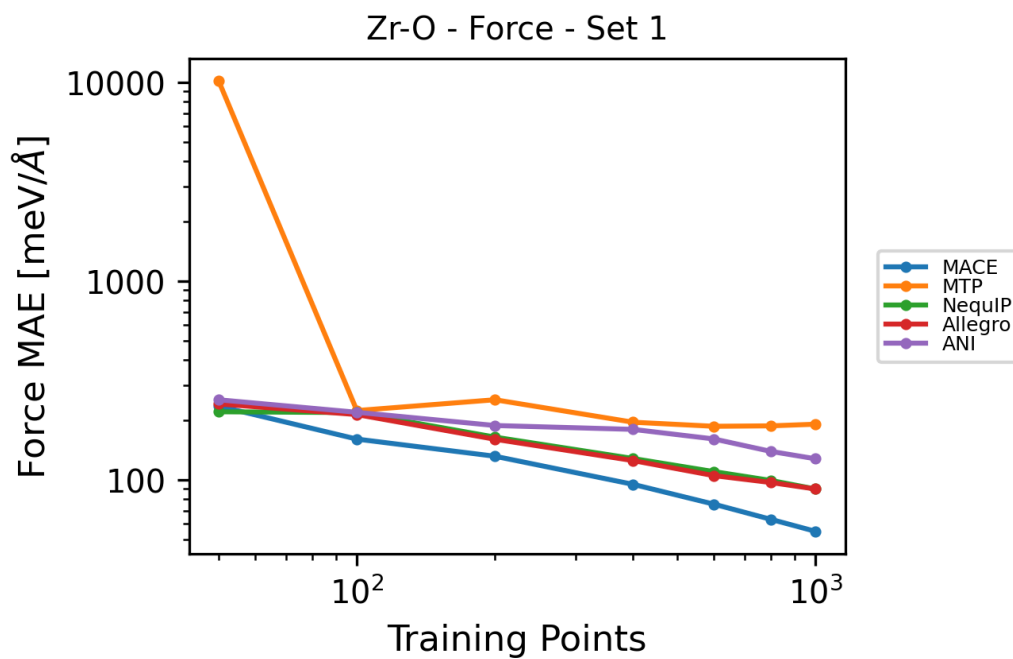
Figure S219. Energy mean absolute error vs training points for Zr-O, Set 2. Unit: meV/atom.
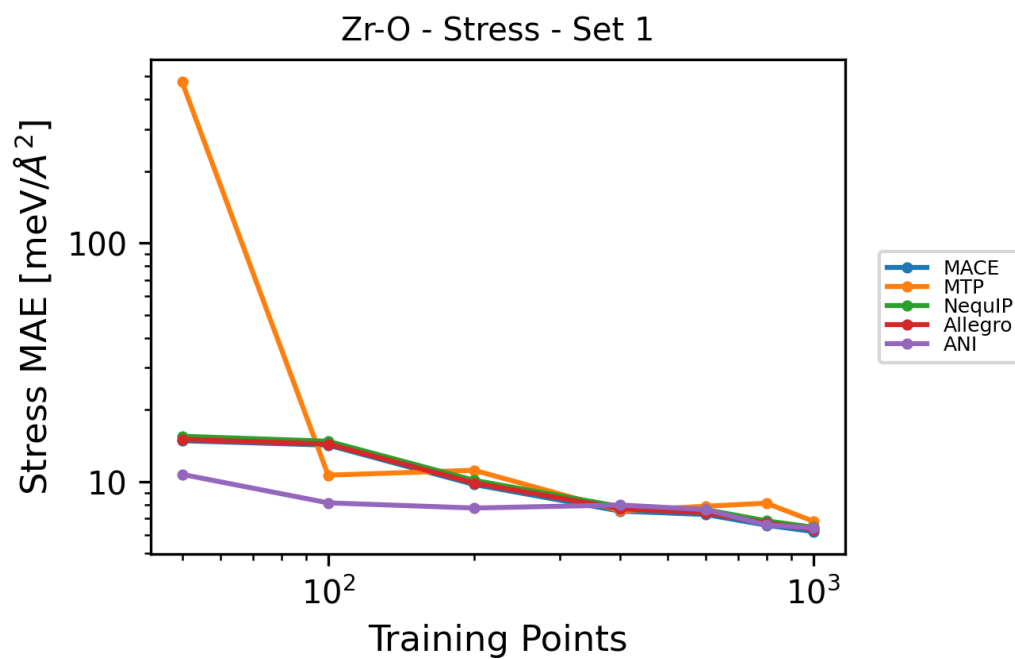
Figure S220. Energy mean absolute error vs training points for Zr-O, Set 2. Unit: meV/atom.
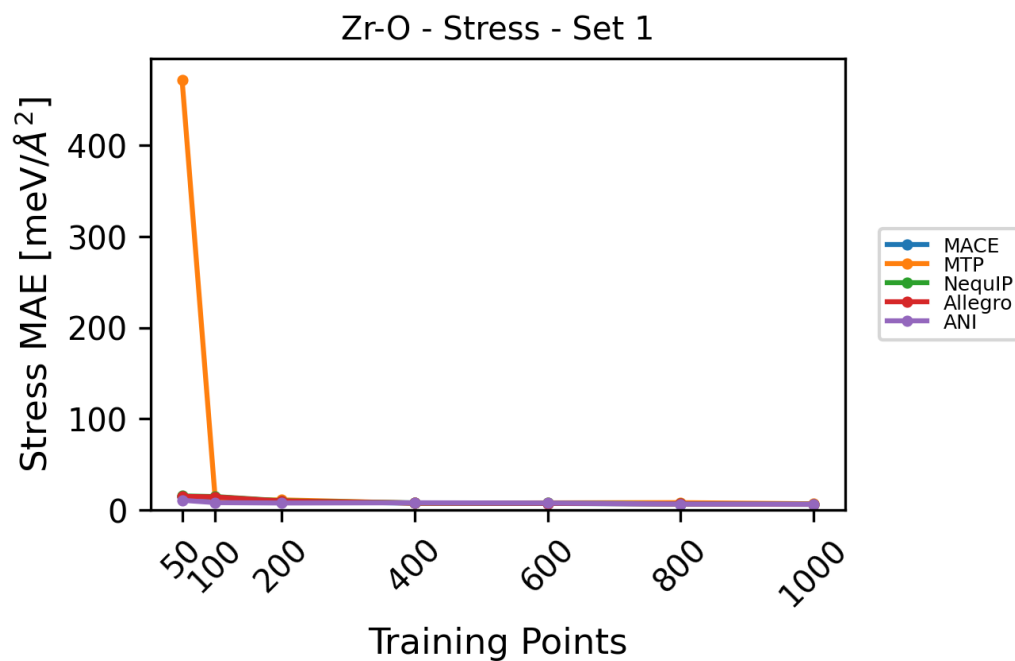
Figure S221. Force mean absolute error vs training points for Zr-O, Set 2. Unit: meV/Å.

Figure S222. Force mean absolute error vs training points for Zr-O, Set 2. Unit: meV/Å.

Figure S223. Stress mean absolute error vs training points for Zr-O, Set 2. Unit: meV/Å².

Figure S224. Stress mean absolute error vs training points for Zr-O, Set 2. Unit: meV/Å².

Figure S225. Energy mean absolute error vs training points for Zr-O, Set 3. Unit: meV/atom.

Figure S226. Energy mean absolute error vs training points for Zr-O, Set 3. Unit: meV/atom.

Figure S227. Force mean absolute error vs training points for Zr-O, Set 3. Unit: meV/Å.
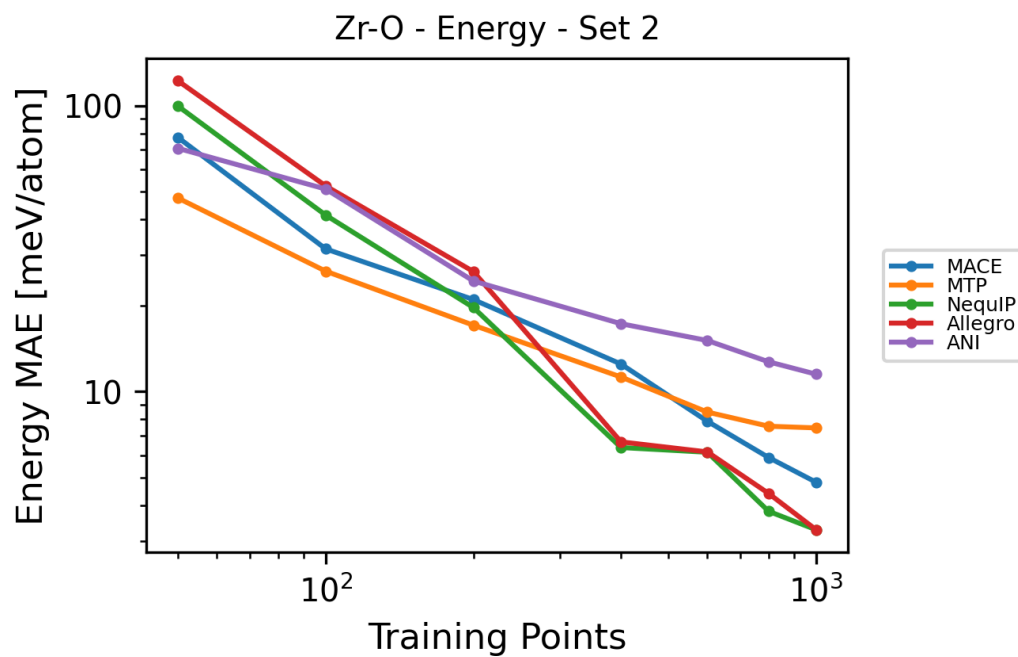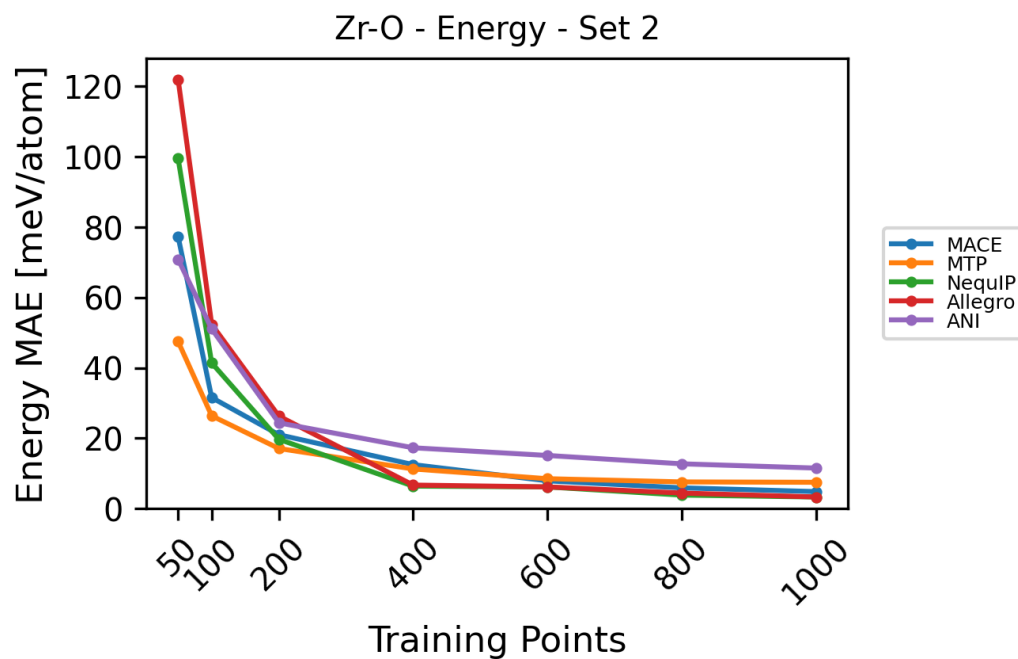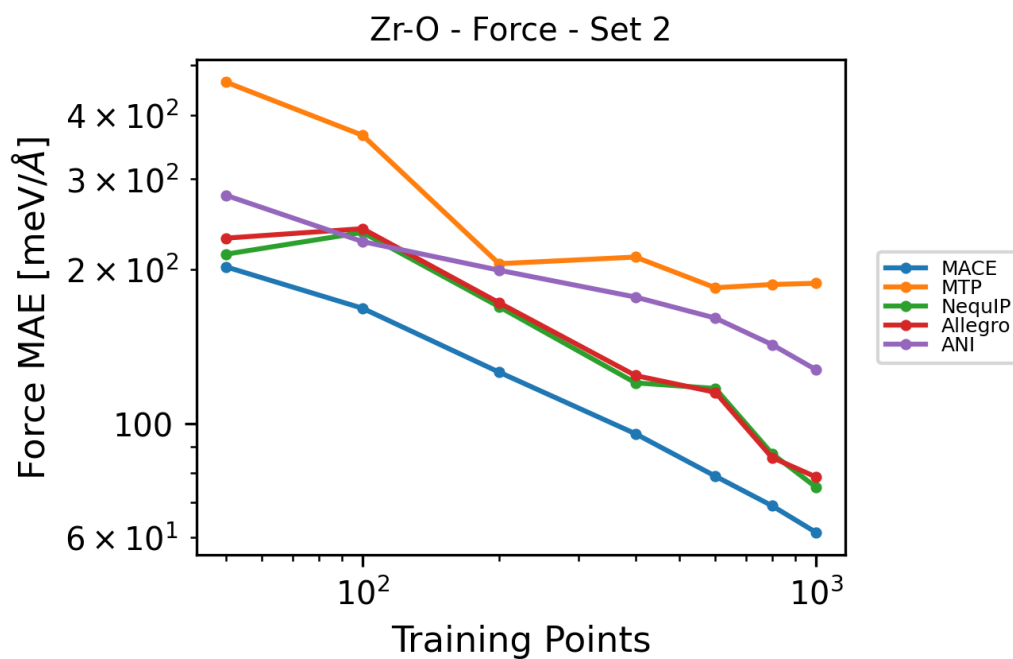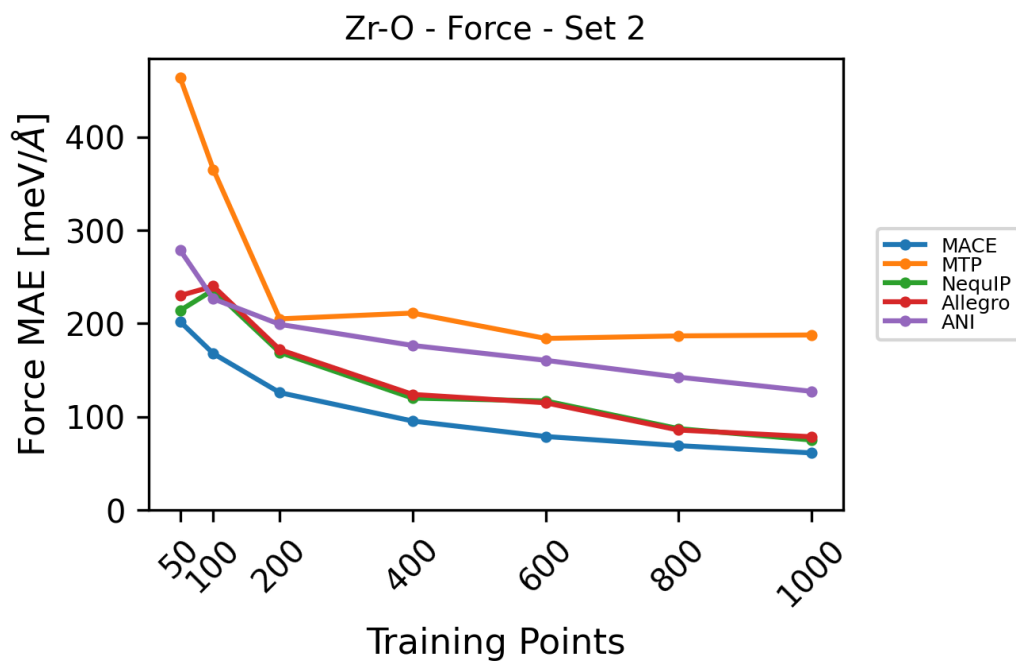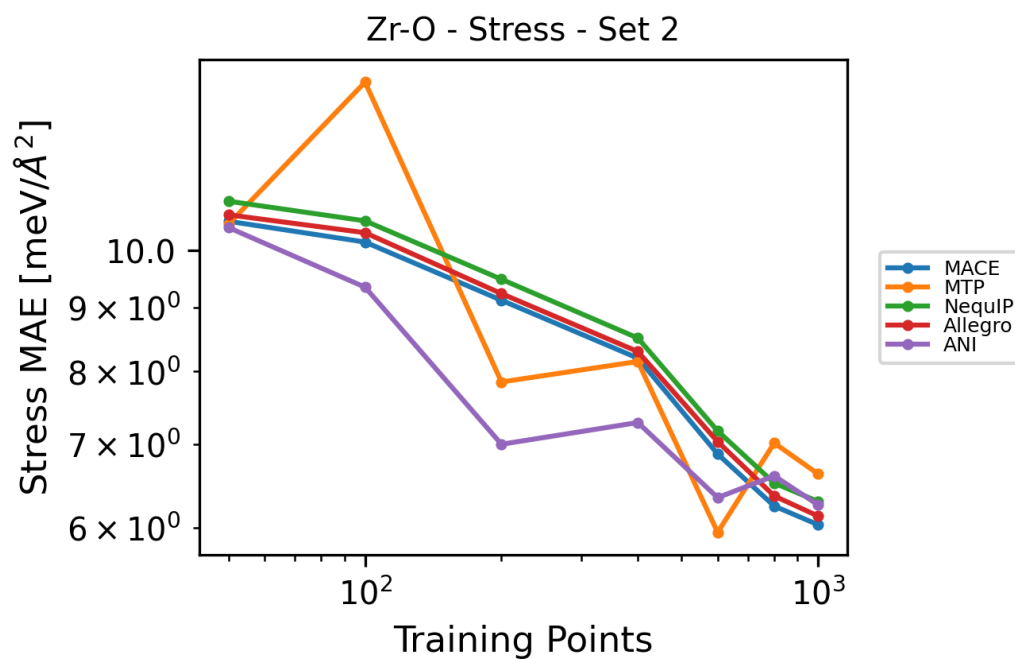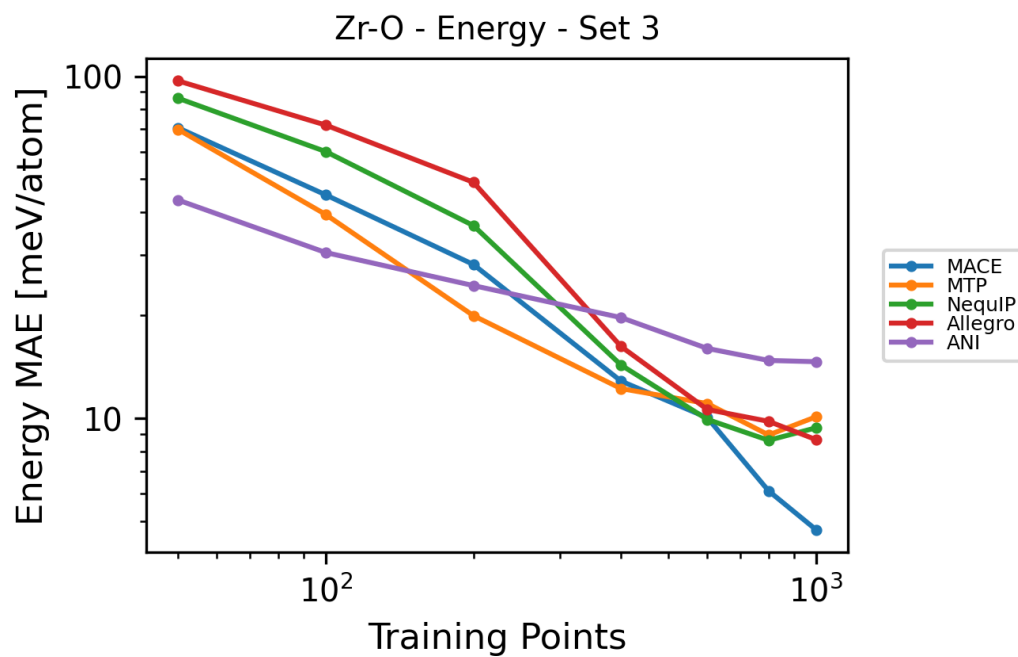
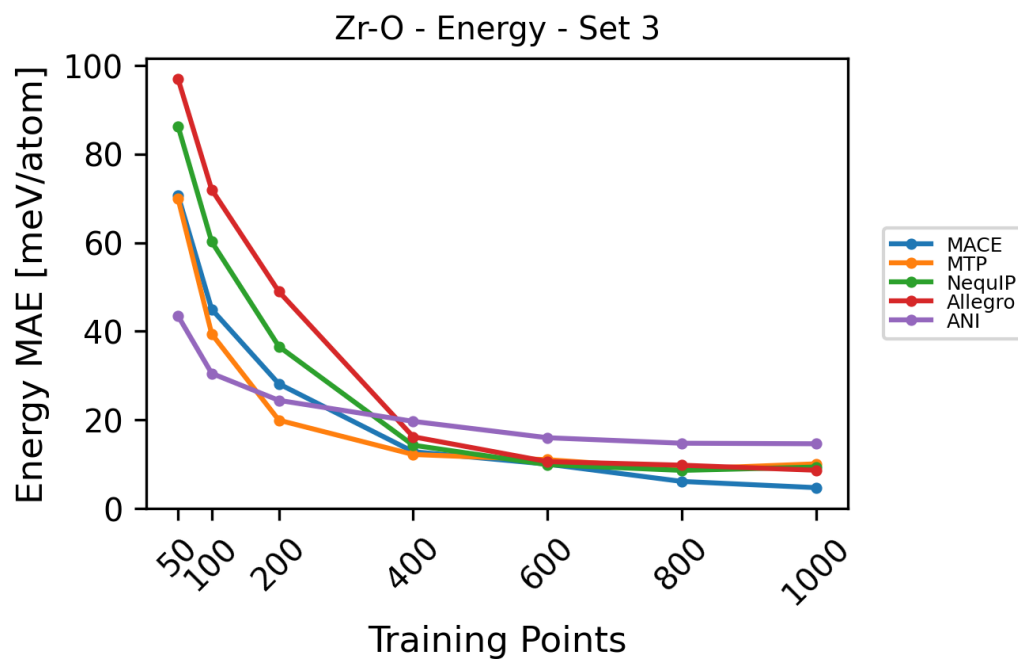**Figure S228.** Force mean absolute error vs training points for Zr-O, Set 3. Unit: meV/Å.

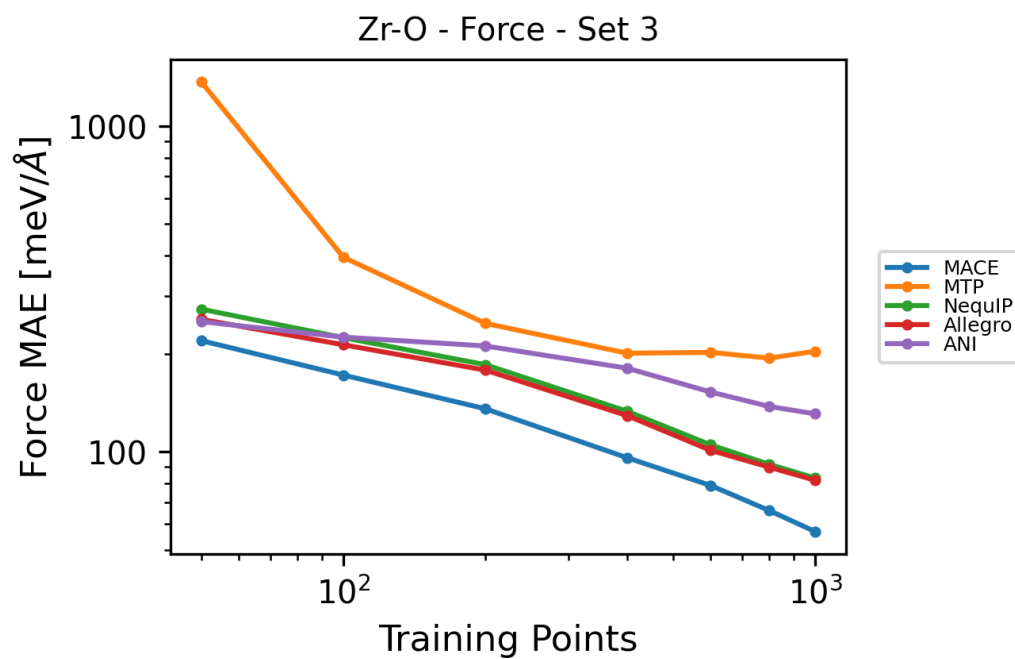**Figure S229.** Stress mean absolute error vs training points for Zr-O, Set 3. Unit: meV/Å².

Figure S230. Stress mean absolute error vs training points for Zr-O, Set 3. Unit: meV/Å².

Figure S231. Energy mean absolute error vs training points for Zr-O, Set mean. Unit: meV/atom.
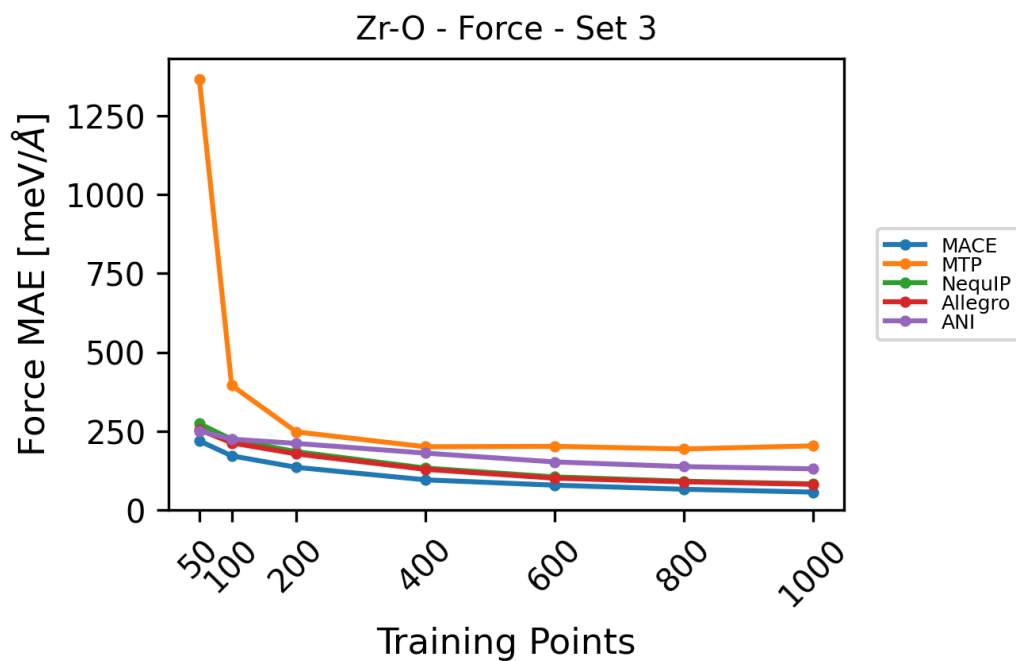
Figure S232. Energy mean absolute error vs training points for Zr-O, Set mean. Unit: meV/atom.
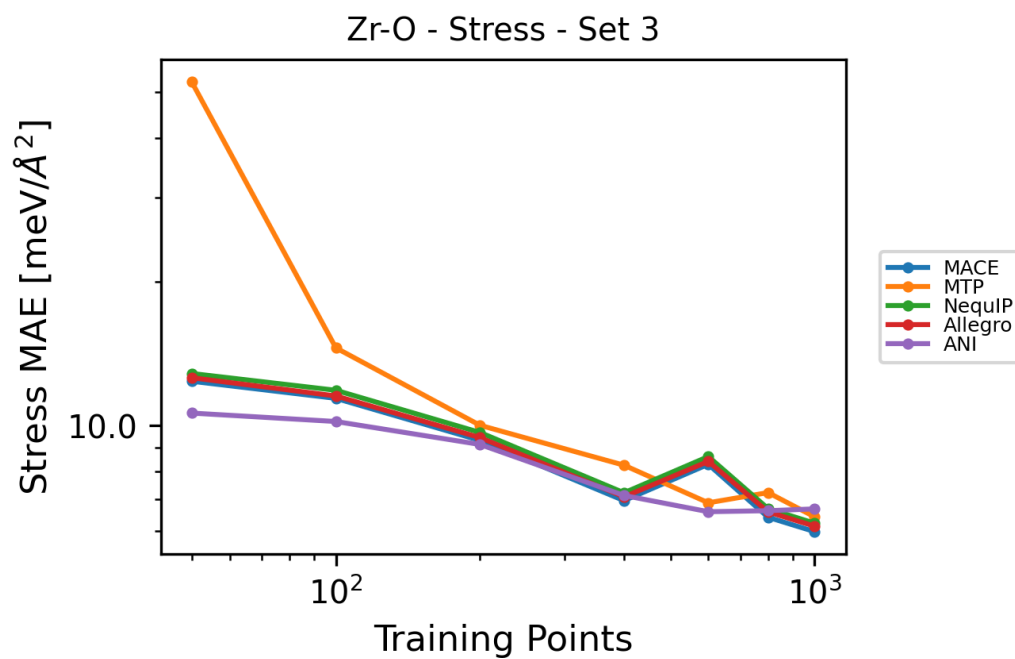
Figure S233. Force mean absolute error vs training points for Zr-O, Set mean. Unit: meV/Å.
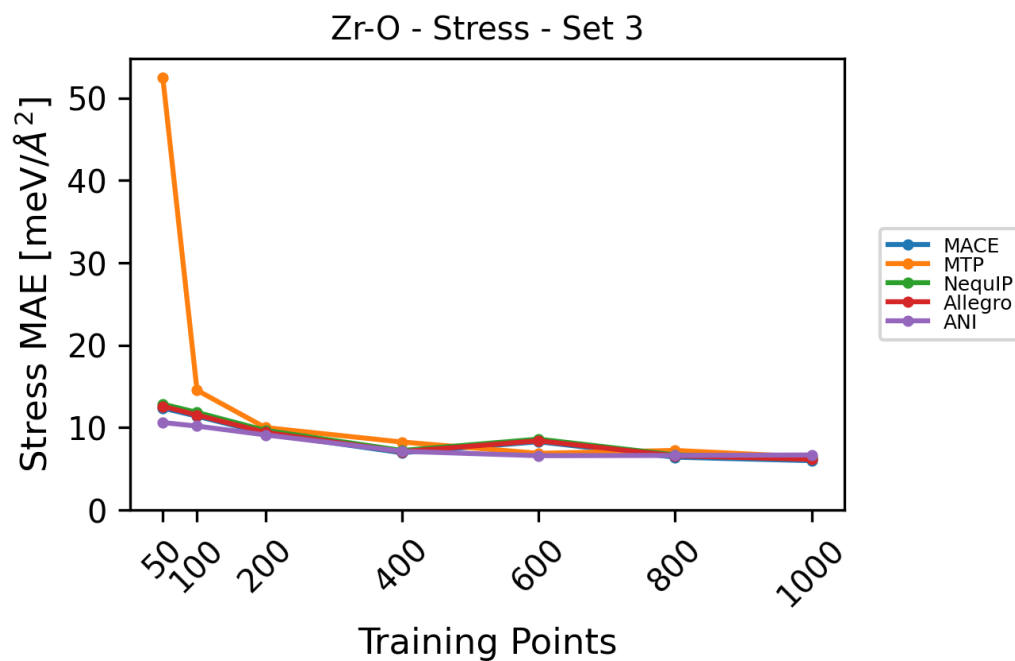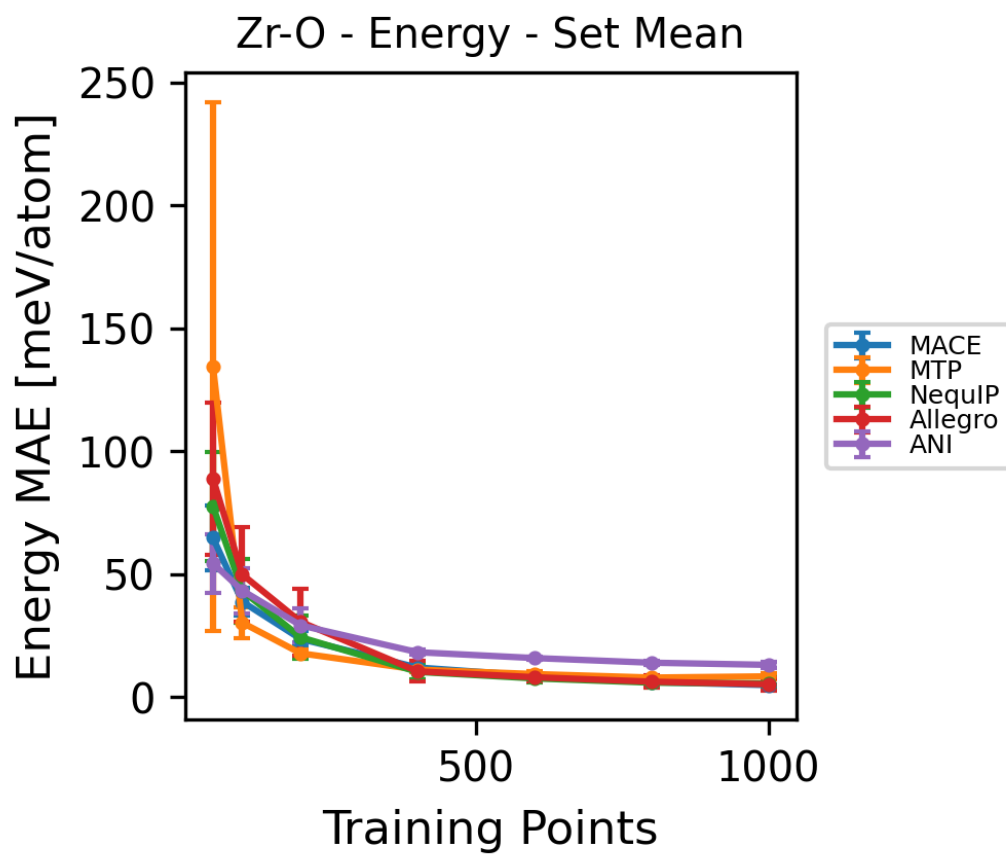
Figure S234. Force mean absolute error vs training points for Zr-O, Set mean. Unit: meV/Å.
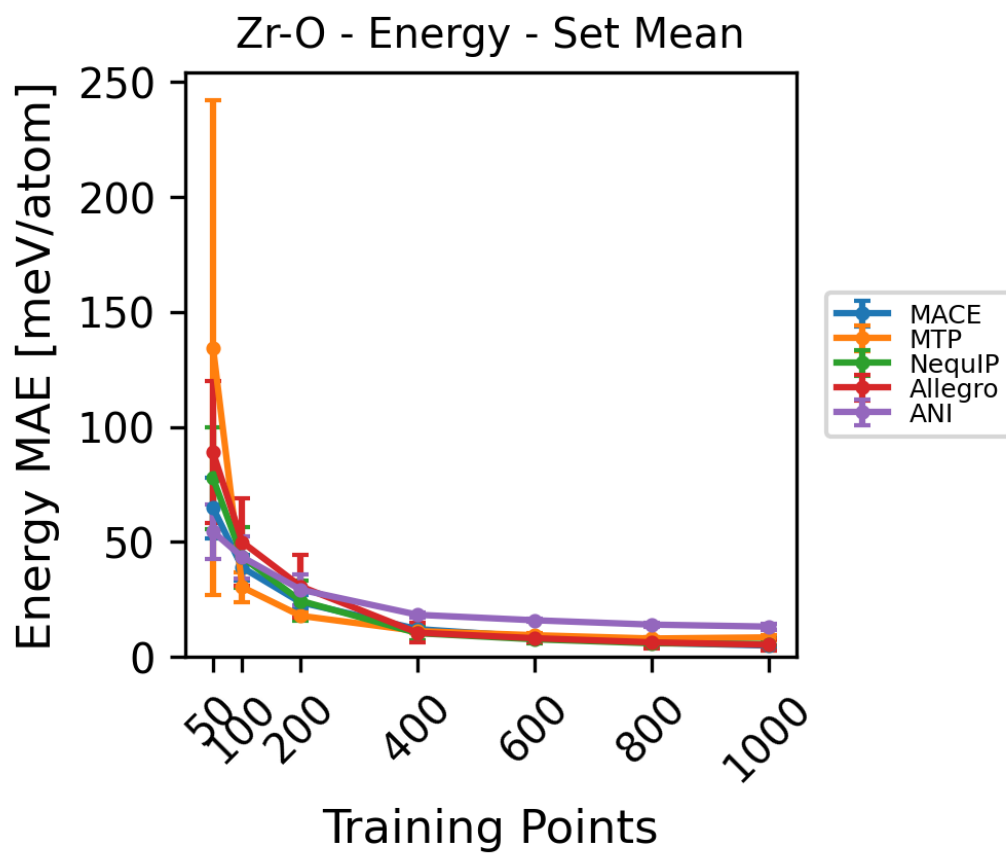
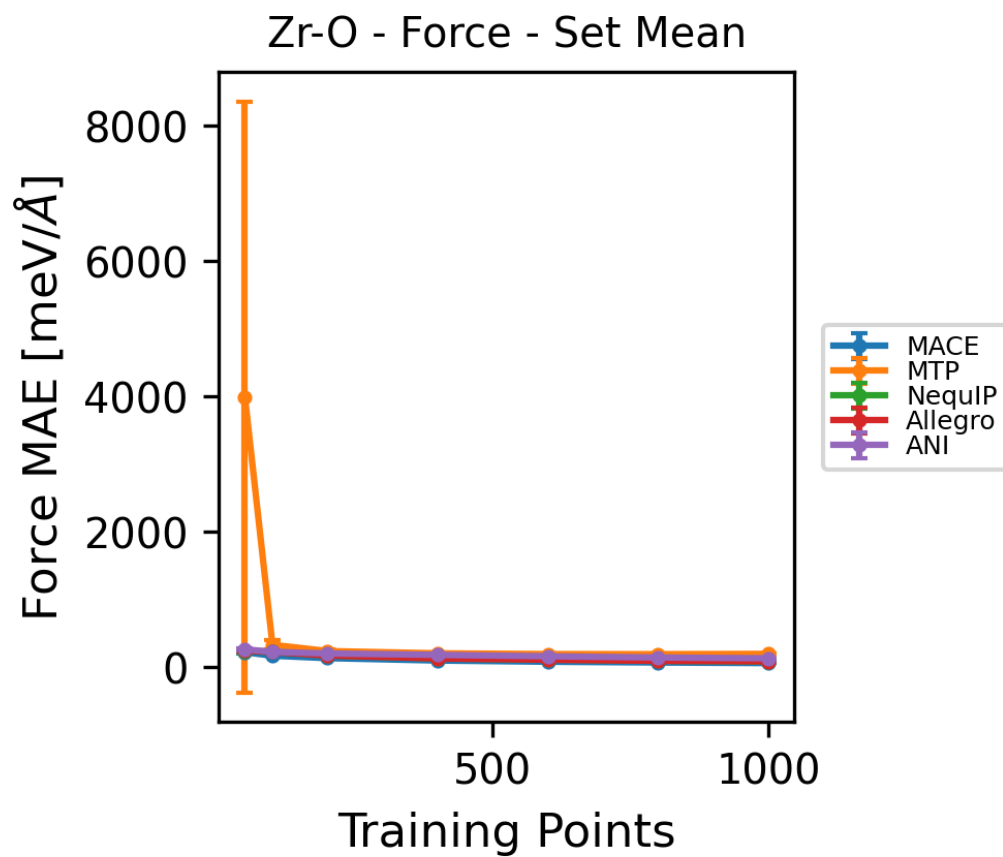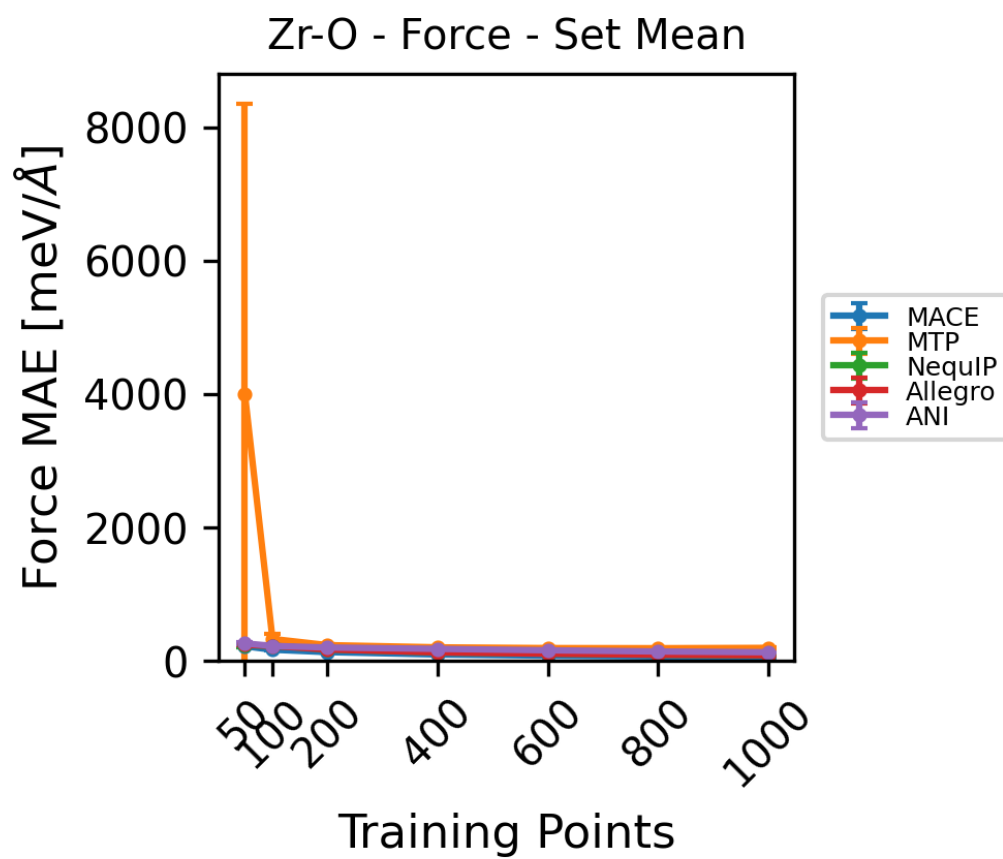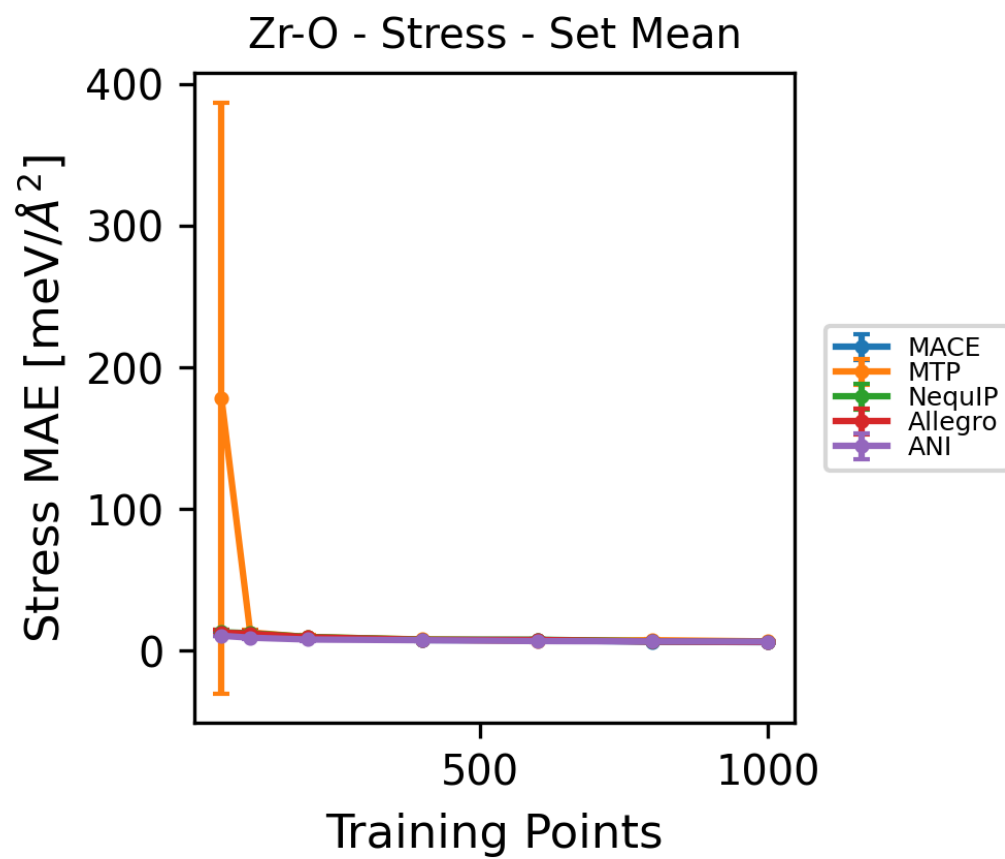**Figure S235.** Stress mean absolute error vs training points for Zr-O, Set mean. Unit: meV/Å².

Figure S236. Stress mean absolute error vs training points for Zr-O, Set mean. Unit: meV/Å².

Training Errors (Energy, Force, Stresses)

Figure S237. Mean absolute error across energy, force, and stress for various datasets at 100 training points (Set 1).

Figure S238. Mean absolute error across energy, force, and stress for various datasets at 1000 training points (Set 1).

Figure S239. Mean absolute error across energy, force, and stress for various datasets at 200 training points (Set 1).

Figure S240. Mean absolute error across energy, force, and stress for various datasets at 400 training points (Set 1).

Figure S241. Mean absolute error across energy, force, and stress for various datasets at 50 training points (Set 1).

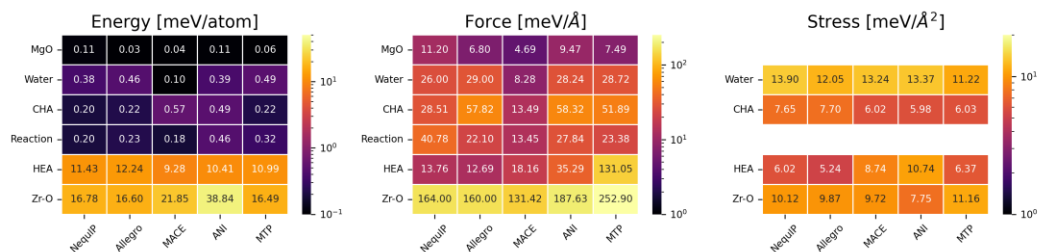**Figure S242.** Mean absolute error across energy, force, and stress for various datasets at 600 training points (Set 1).

Figure S243. Mean absolute error across energy, force, and stress for various datasets at 800 training points (Set 1).
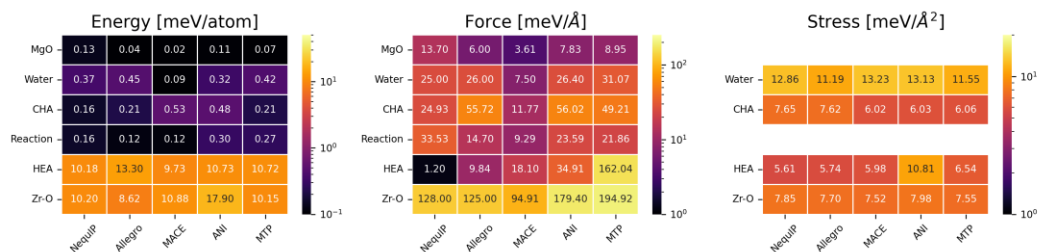
Figure S244. Mean absolute error across energy, force, and stress for various datasets at 100 training points (Set 2).
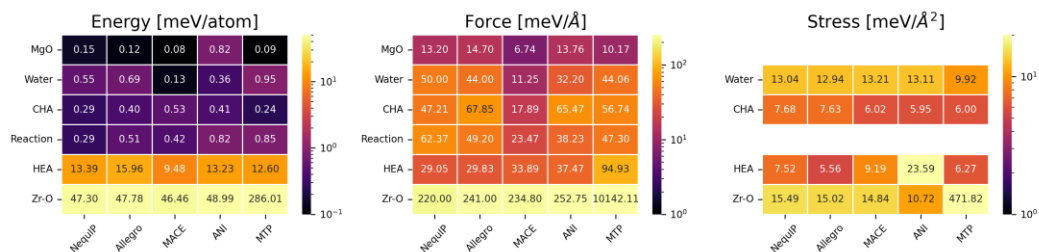
Figure S245. Mean absolute error across energy, force, and stress for various datasets at 1000 training points (Set 2).
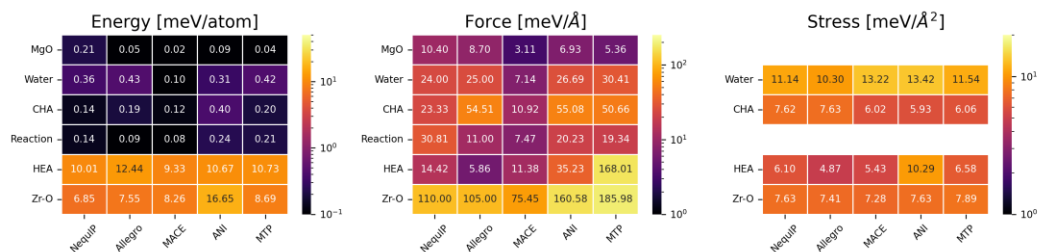
Figure S246. Mean absolute error across energy, force, and stress for various datasets at 200 training points (Set 2).
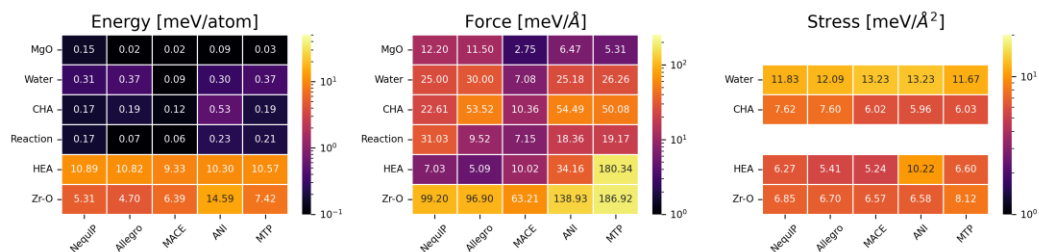
Figure S247. Mean absolute error across energy, force, and stress for various datasets at 400 training points (Set 2).

Figure S248. Mean absolute error across energy, force, and stress for various datasets at 50 training points (Set 2).
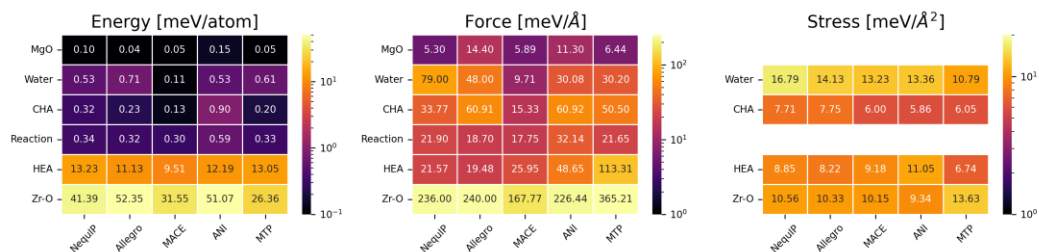
Figure S249. Mean absolute error across energy, force, and stress for various datasets at 600 training points (Set 2).
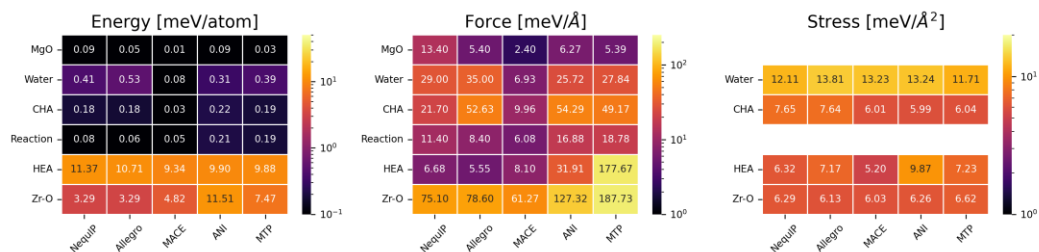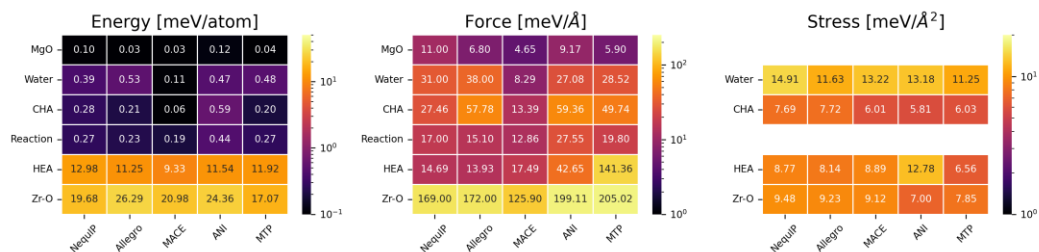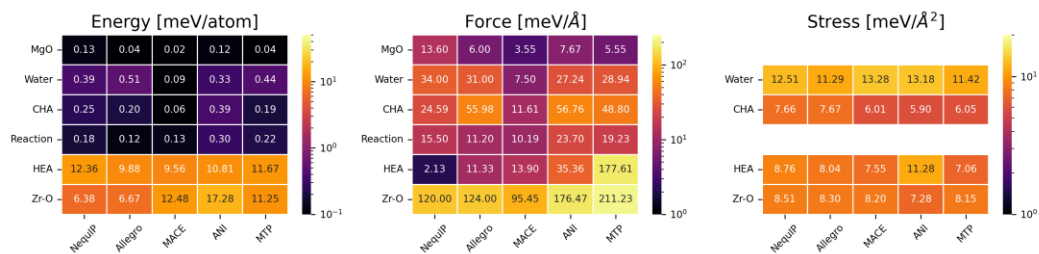
Figure S250. Mean absolute error across energy, force, and stress for various datasets at 800 training points (Set 2).
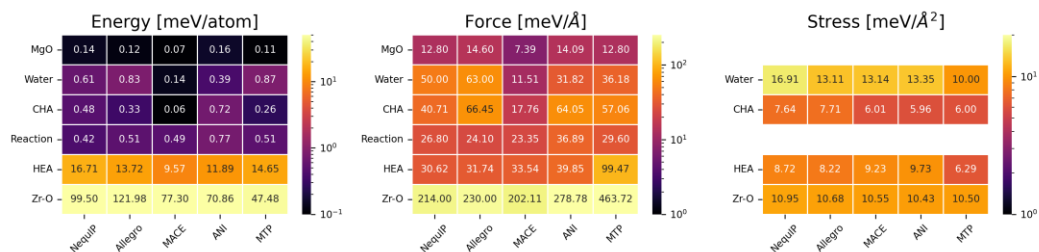
Figure S251. Mean absolute error across energy, force, and stress for various datasets at 100 training points (Set 3).
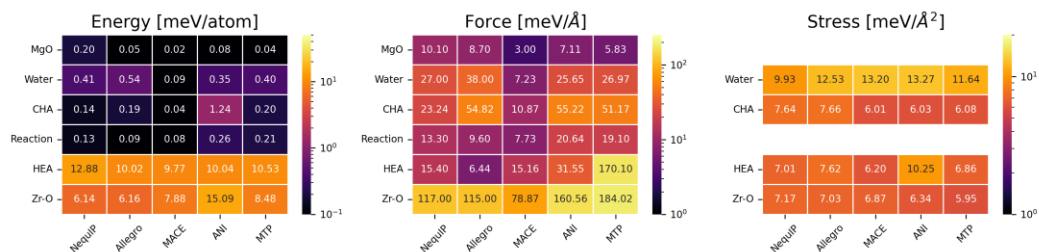
Figure S252. Mean absolute error across energy, force, and stress for various datasets at 1000 training points (Set 3).

Figure S253. Mean absolute error across energy, force, and stress for various datasets at 200 training points (Set 3).
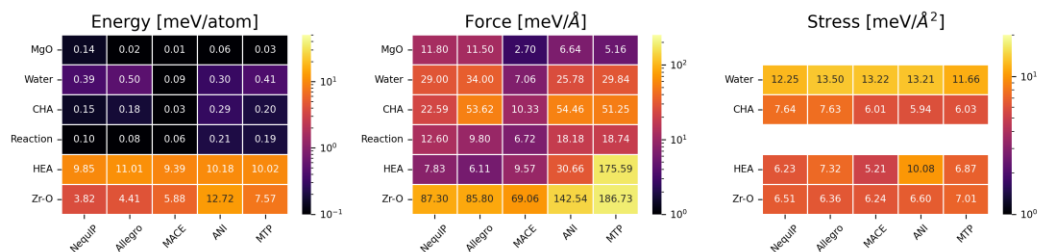
Figure S254. Mean absolute error across energy, force, and stress for various datasets at 400 training points (Set 3).
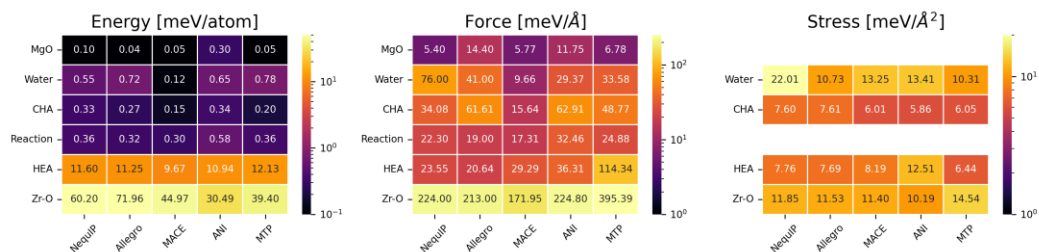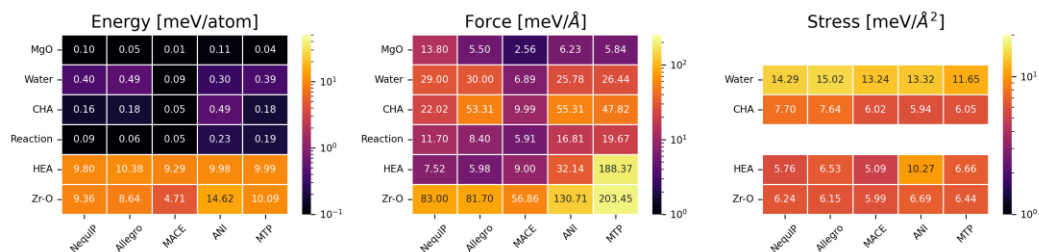
Figure S255. Mean absolute error across energy, force, and stress for various datasets at 50 training points (Set 3).
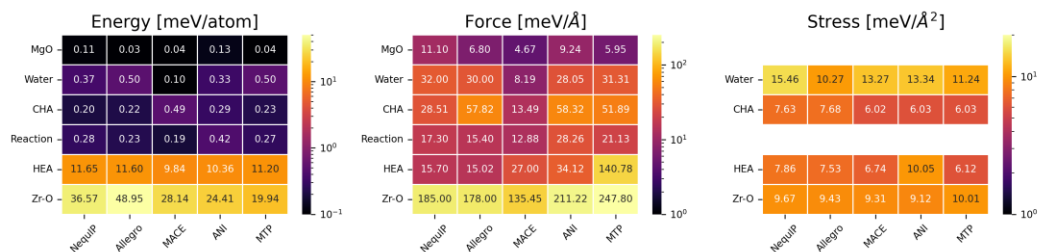
Figure S256. Mean absolute error across energy, force, and stress for various datasets at 600 training points (Set 3).

Figure S257. Mean absolute error across energy, force, and stress for various datasets at 800 training points (Set 3).
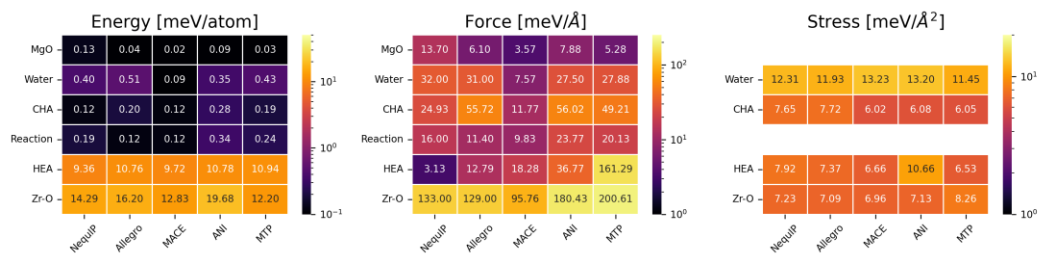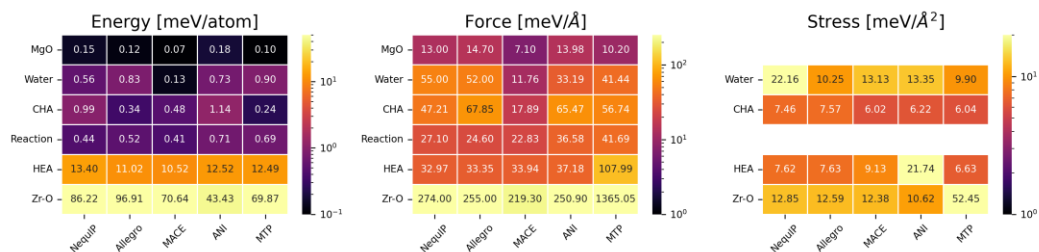
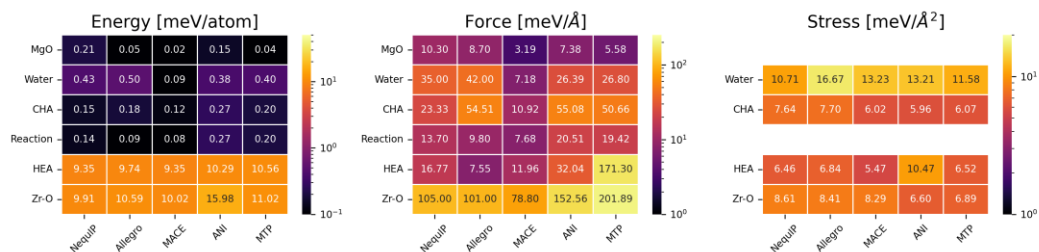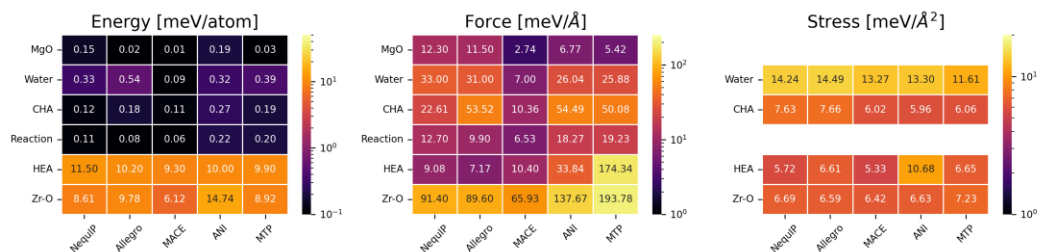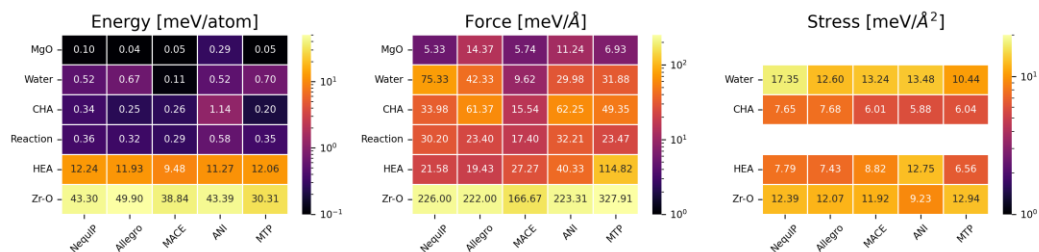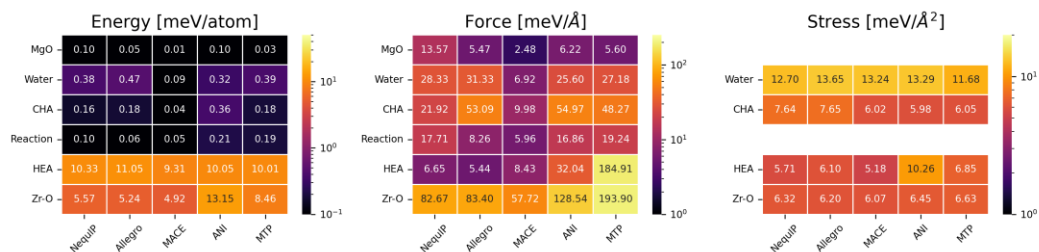**Figure S258.** Mean absolute error across energy, force, and stress for various datasets at 100 training points (Set mean).

Figure S259. Mean absolute error across energy, force, and stress for various datasets at 1000 training points (Set mean).
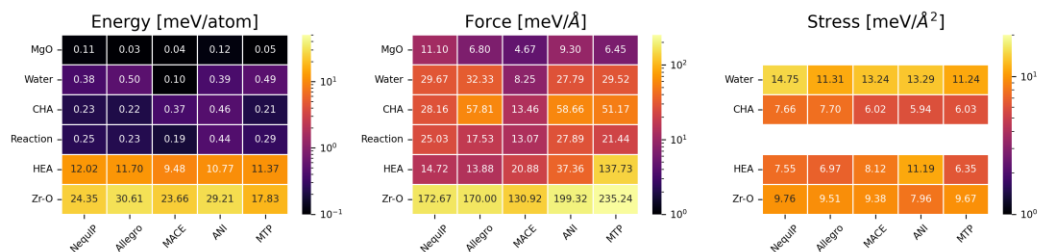
Figure S260. Mean absolute error across energy, force, and stress for various datasets at 200 training points (Set mean).

Figure S261. Mean absolute error across energy, force, and stress for various datasets at 400 training points (Set mean).

Figure S262. Mean absolute error across energy, force, and stress for various datasets at 50 training points (Set mean).
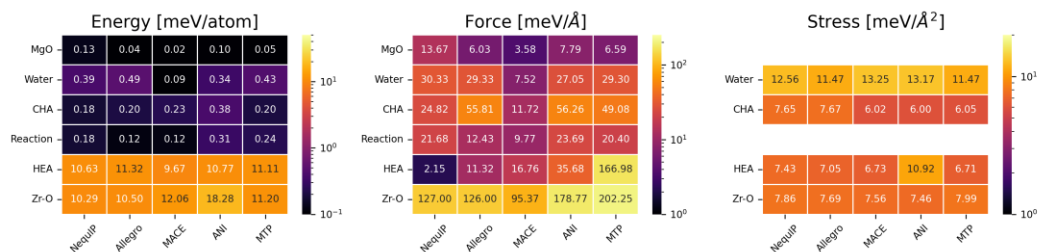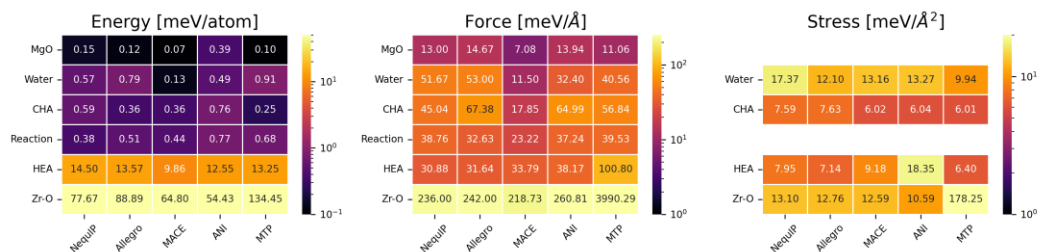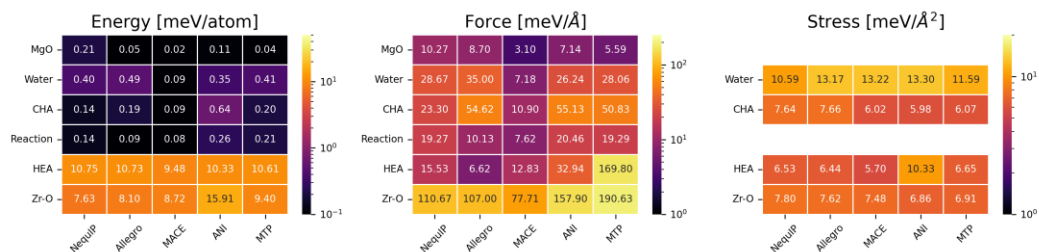
Figure S263. Mean absolute error across energy, force, and stress for various datasets at 600 training points (Set mean).
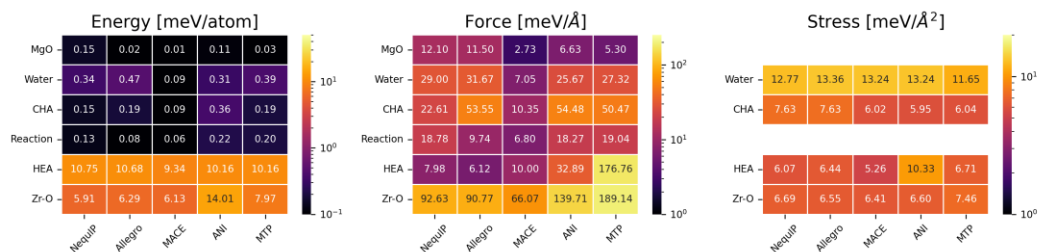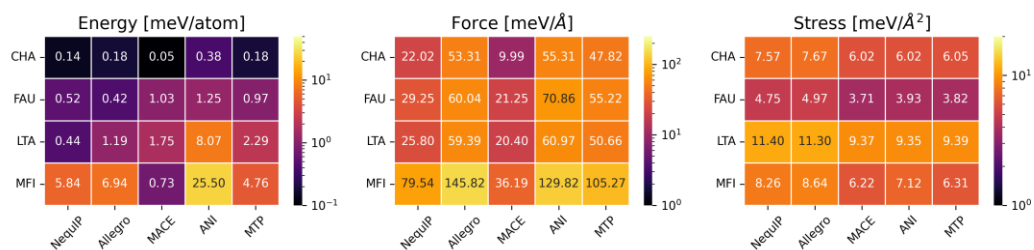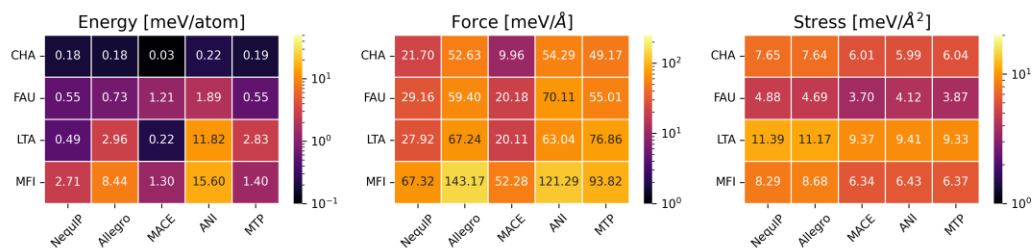
Figure S264. Mean absolute error across energy, force, and stress for various datasets at 800 training points (Set mean).
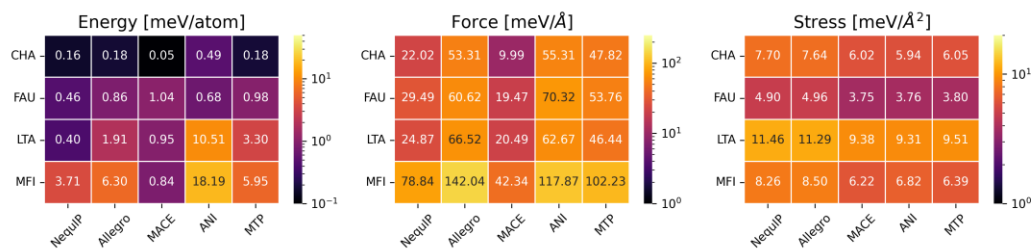
Zeolite Transferability

Figure S265. Error across energy, force, and stress for CHA, FAU, LTA, and MFI zeolites at 1000 training points (Set 1).
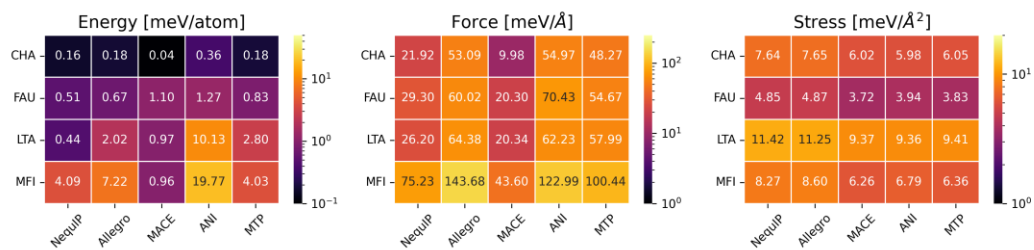
Figure S266. Error across energy, force, and stress for CHA, FAU, LTA, and MFI zeolites at 1000 training points (Set 2).
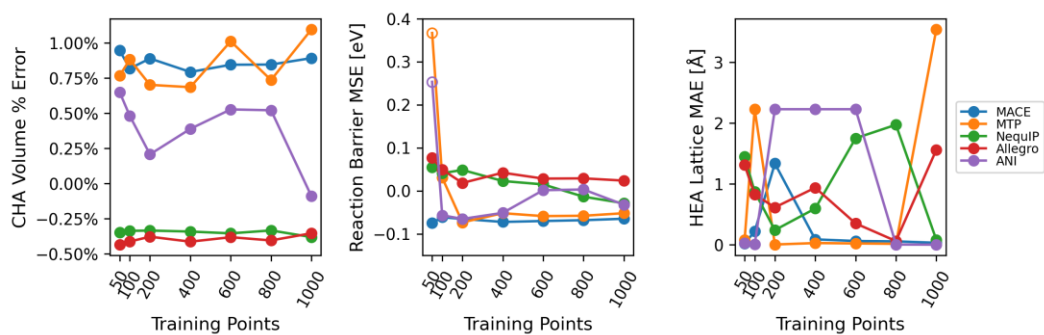
Figure S267. Error across energy, force, and stress for CHA, FAU, LTA, and MFI zeolites at 1000 training points (Set 3).
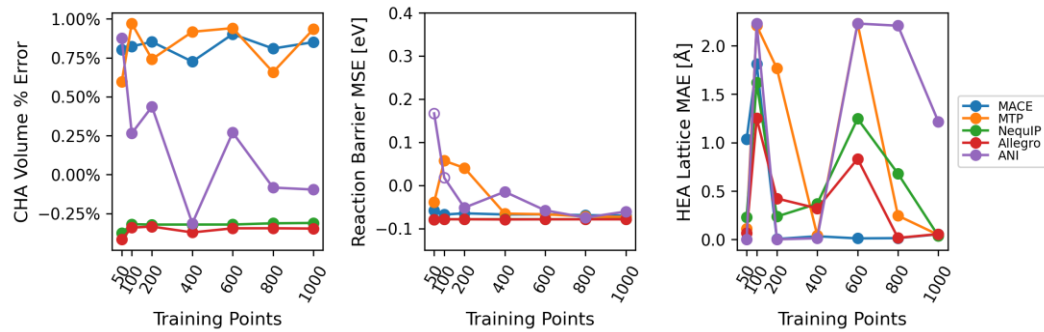
Figure S268. Error across energy, force, and stress for CHA, FAU, LTA, and MFI zeolites at 1000 training points (Set mean).
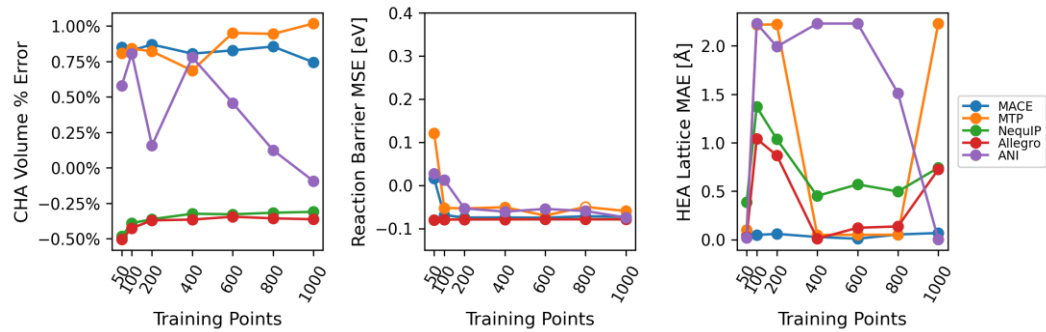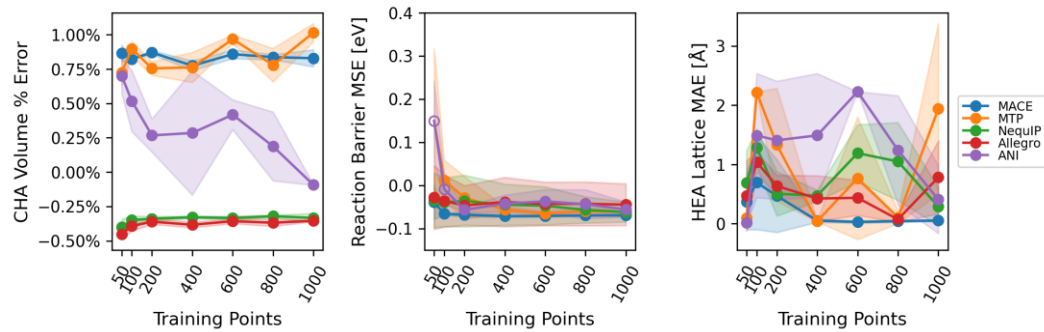
Observable Errors

Figure S269. Prediction error in derived observables: CHA volume, HEA lattice constants, and BM barriers (Set 1).

Figure S270. Prediction error in derived observables: CHA volume, HEA lattice constants, and BM barriers (Set 2).

Figure S271. Prediction error in derived observables: CHA volume, HEA lattice constants, and BM barriers (Set 3).

Figure S272. Prediction error in derived observables: CHA volume, HEA lattice constants, and BM barriers (Set mean).