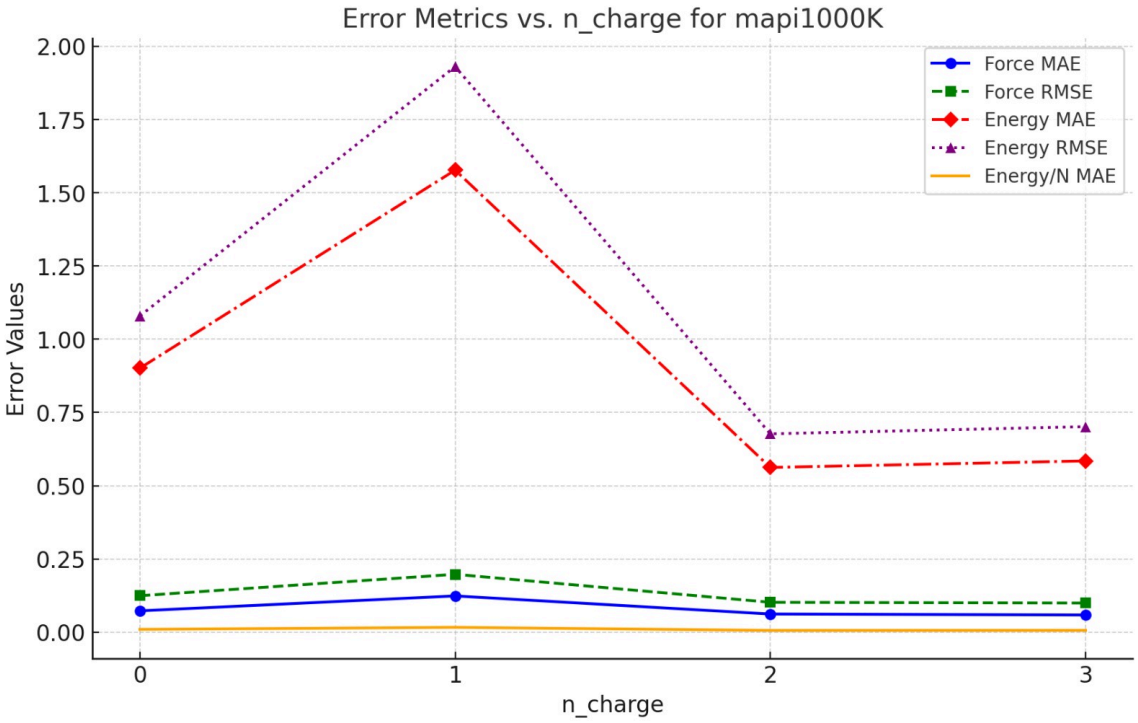
Comparative Analysis of NequIP and NequIP-LR - III

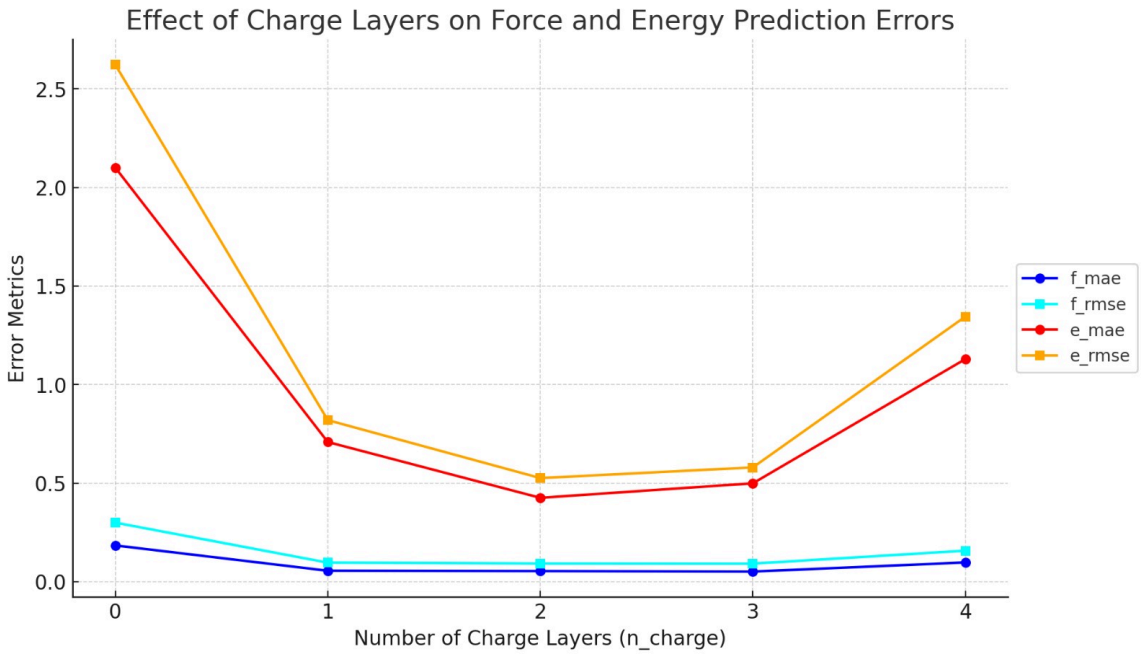
MAPI- 1000K

A) Effect of increasing the number of charge layers-total_layers3



- Adding charge-encoding reduces the errors
- It has been observed that even when we scale the model or prune it, the charge layers need to be around constant to capture long range interactions

B) Effect of increasing the number of charge layers-total_layers4



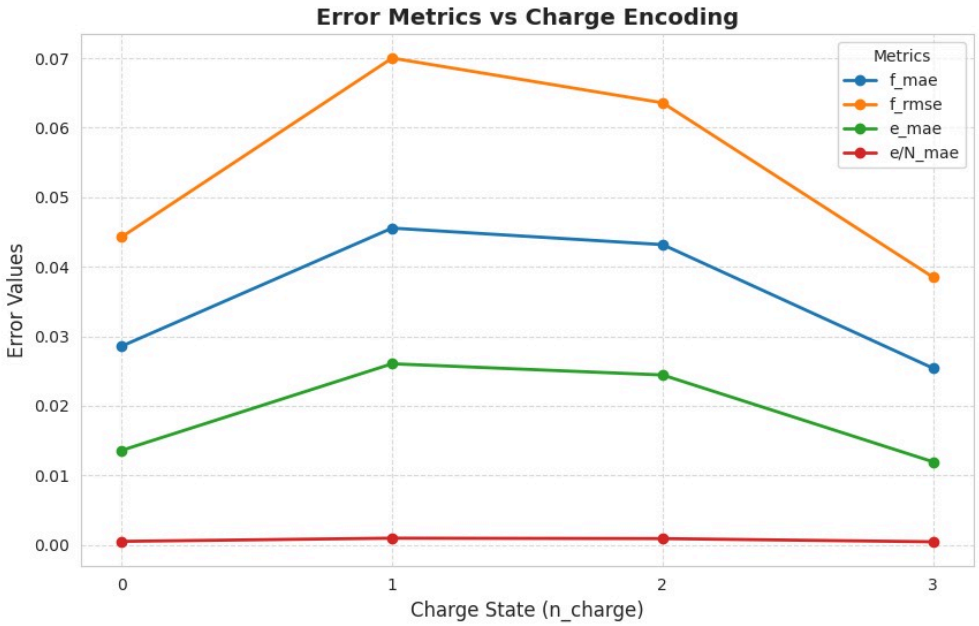
- **Adding charge-encoding reduces the errors considerably**
- **We again observe that even if we scale the total layers , adding some charge encoding (2 layers) considerably reduces the errors.**

We observe that a sweet spot of capturing the charge-encoding needs to be found so that performance is increased , using less or more charge layers increases the errors

SCALING IMPROVES THE PERFORMANCE OF NEQUIP , BUT SCALING CHARGE LAYERS ARE NOT HELPFUL

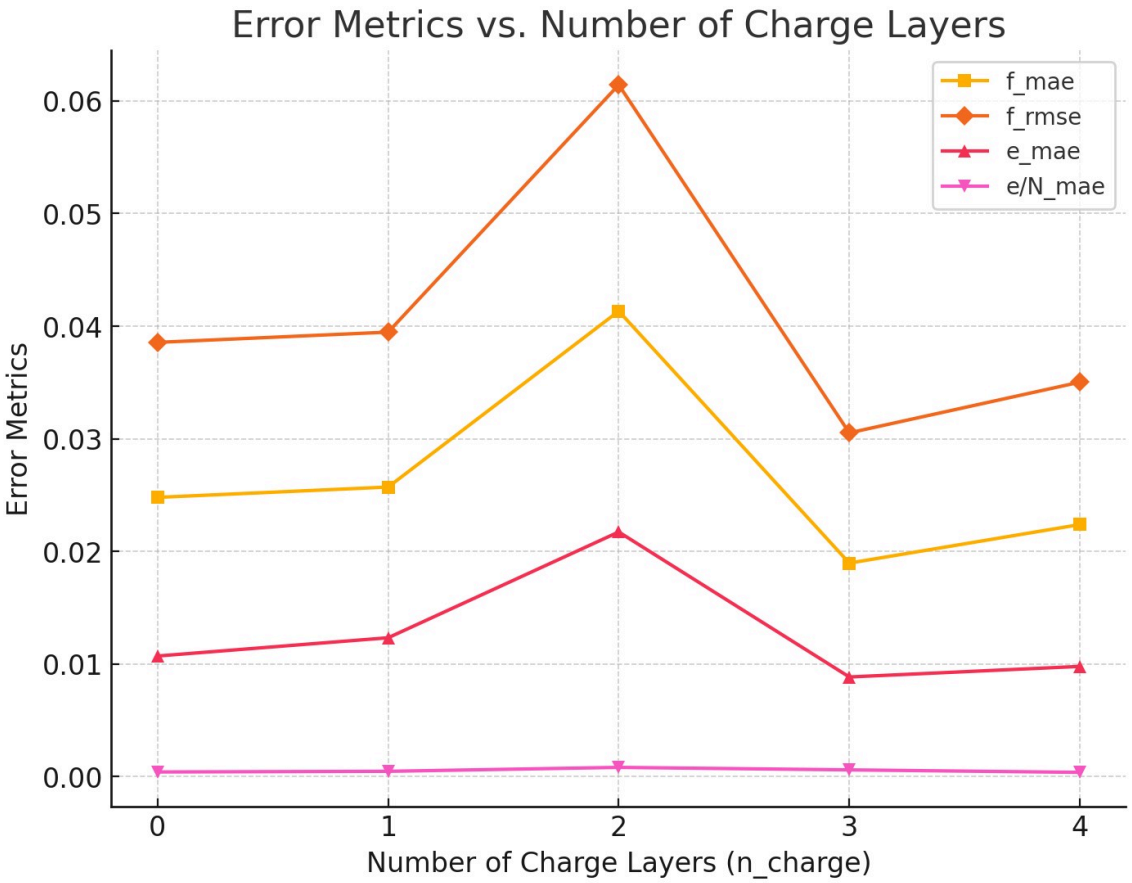
3BPA

C) Effect of increasing the number of charge layers-total_layers3



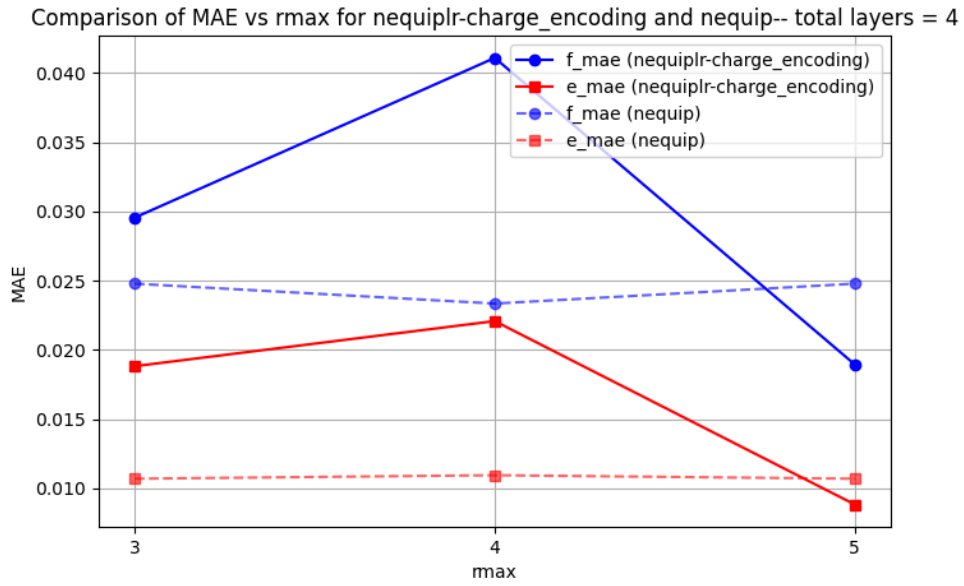
■ The test results with n_total = 3 where all layers are charge layers are better than the original nequip with total_layers = 6 and no charge layers. It shows that smaller nequip-lr models give better results than bigger nequip models .

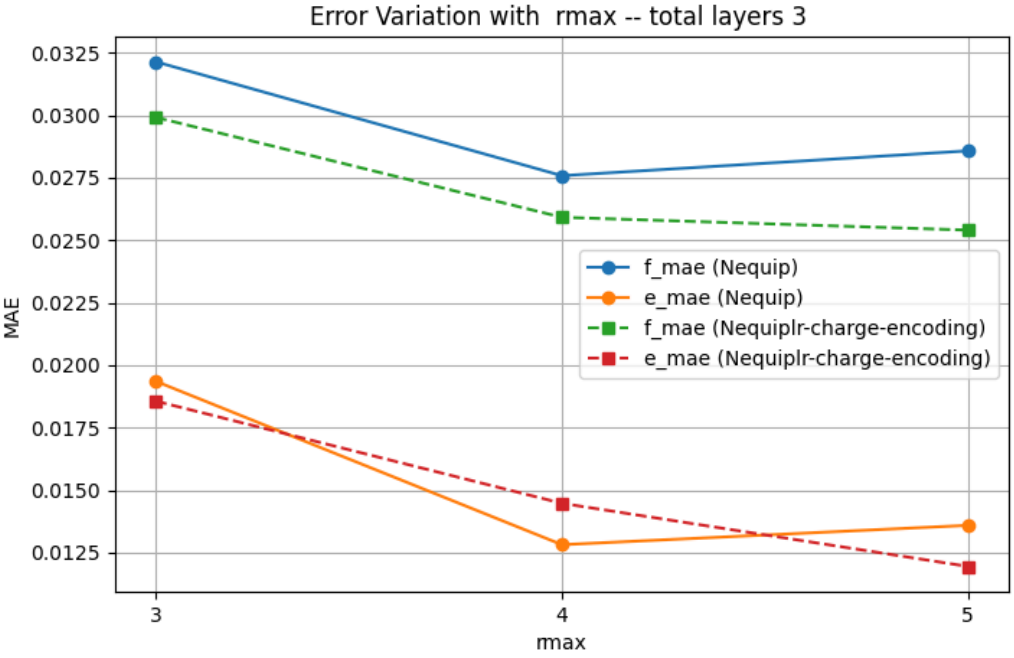
D) Effect of increasing the number of charge layers-total_layers4



■ **As stated before , a constant number of charge layers are helpful to improve the results even if the model is scaled down.**

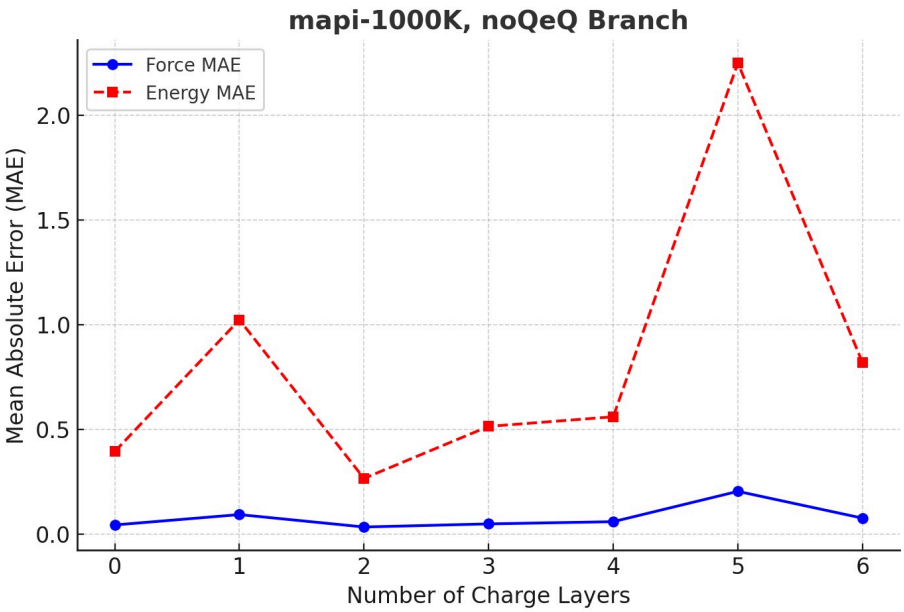
E) Effect of increasing rmax

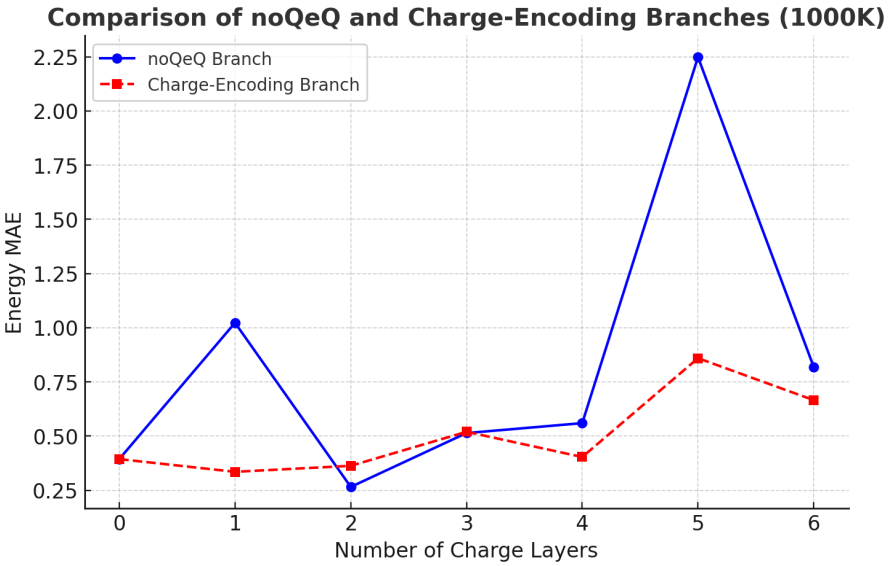




NoQeq branch

A)increasing no of charge layers- mapi 1000K

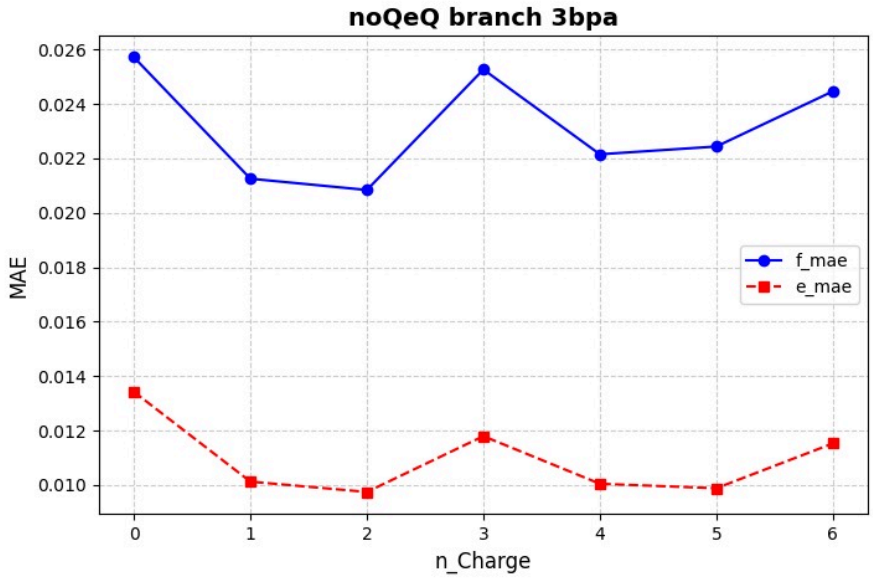




The charge-encoding branch appears more robust in handling charge interactions.

It maintains lower and more stable Energy MAE across different charge layers.

A)increasing no of charge layers- 3bpa



The energy predictions are surprisingly better than force