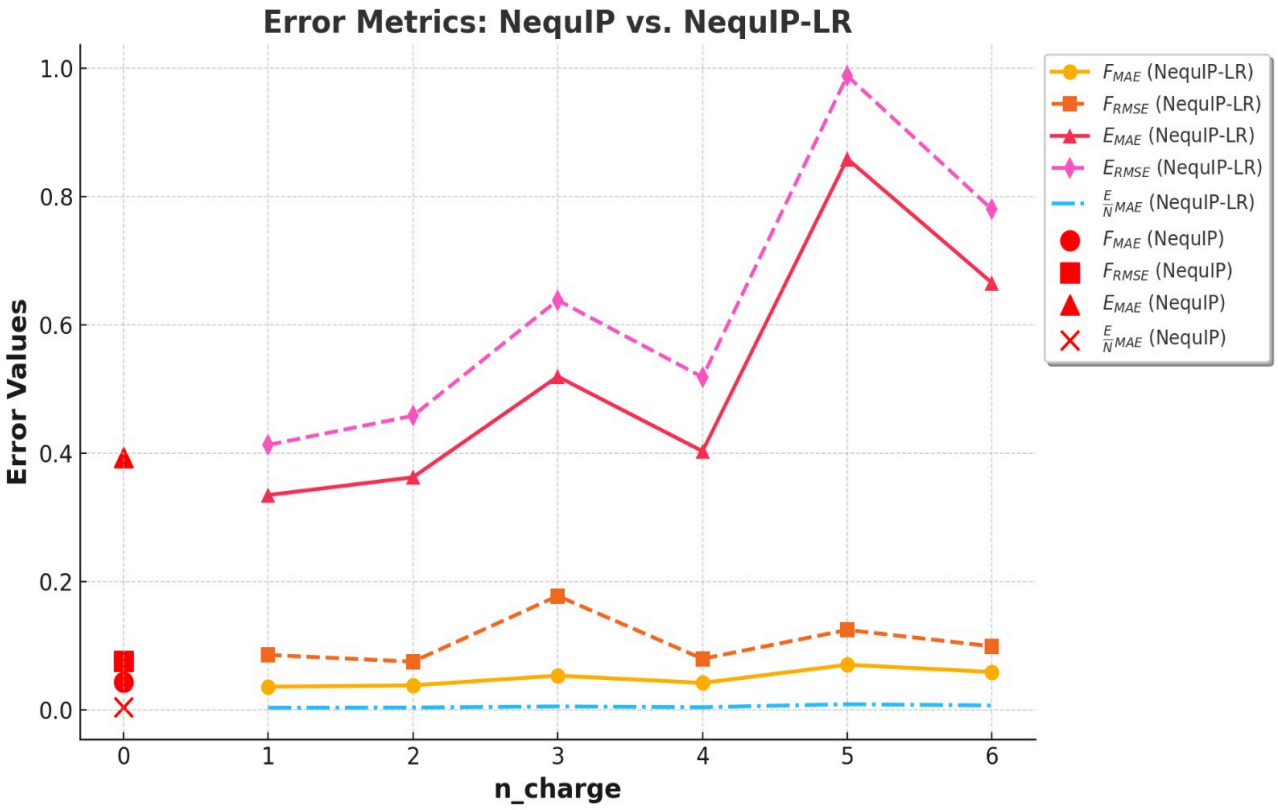
Comparative Analysis of NequIP and NequIP-LR - II

MAPI- 1000K

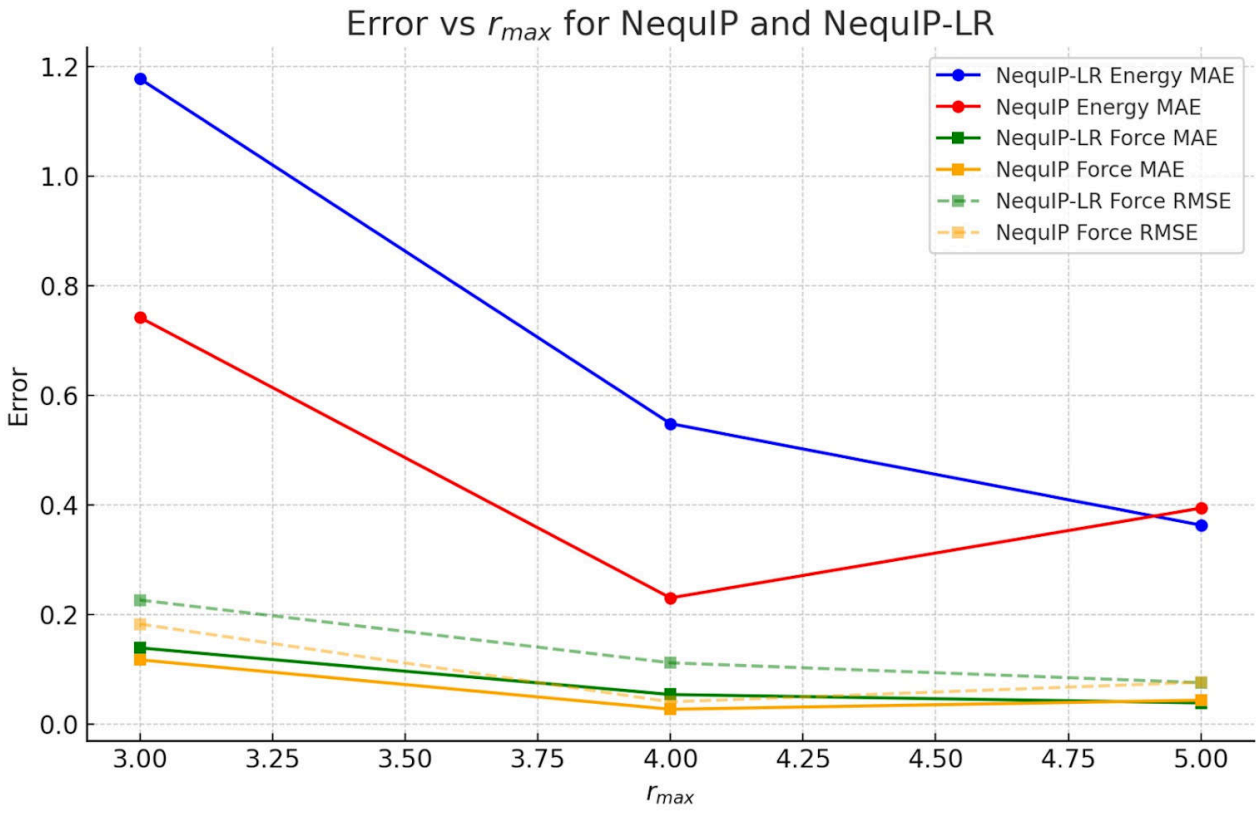
A) Effect of increasing the number of charge layers



- Nequip LR has lower e_mae than Nequipr for n_charge = 1 and n_charge = 2

- F_mae is almost constant as we increase the number of layers , but it is lower than Nequip for the first 2 additions.

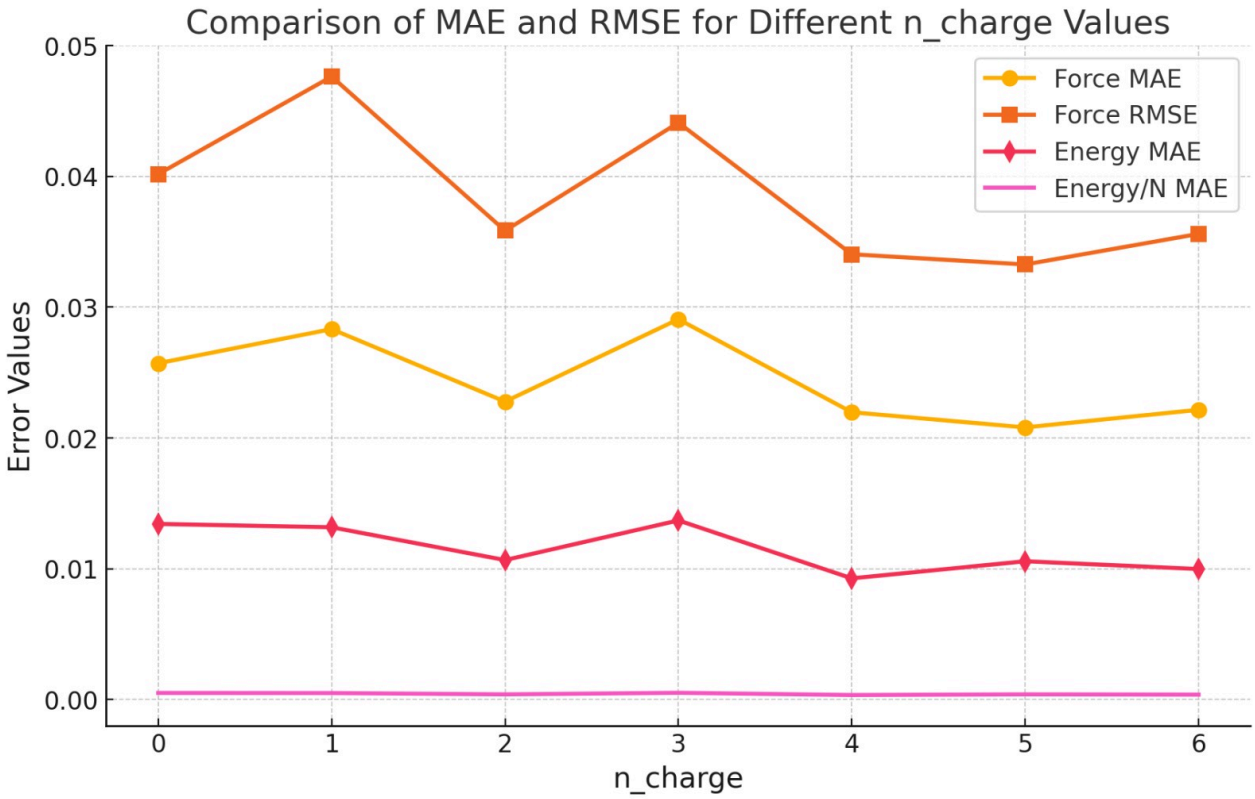
B) Effect of increasing cutoff radius in Nequip-LR



As we keep on increasing the cutoff radius, NequipLR achieves better performance

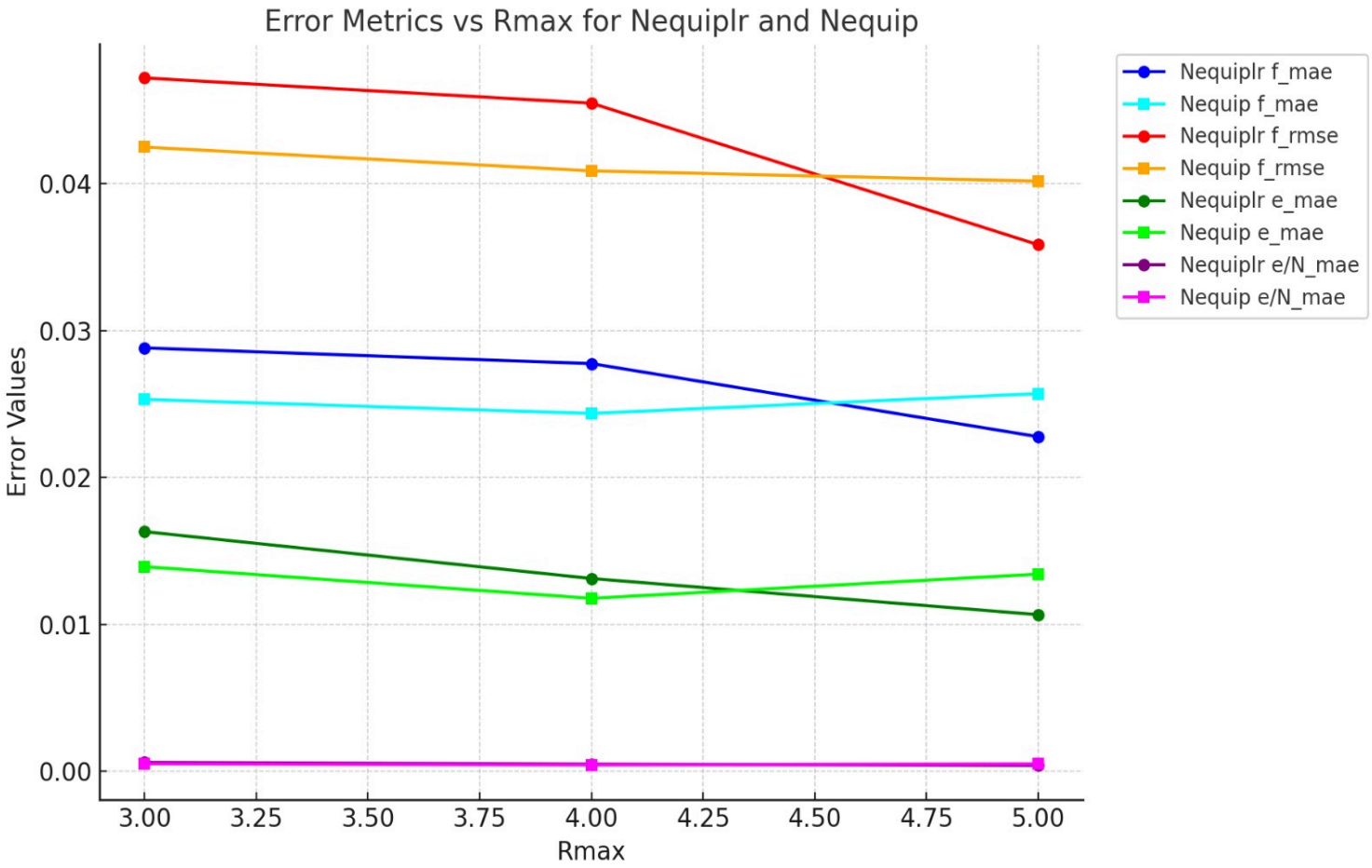
3BPA

A) Effect of increasing the number of charge layers



- Long range interactions are very significant in 3bpa.
- Lowest e_mae is achieved when n_charge = 5, significantly lower than Nequip

B) Effect of increasing cutoff radius in Nequip-LR



- As long range interactions are more significant, the reduction in error in NequipLR is significantly more in 3BPA than in MAPI-1000K, when we increase the cutoff radius to r = 5
- Similar trends are observed for Force.
- But we have seen that changing the number of charge layers affect Forces way lesser than Energy

NO SIGNIFICANT IMPROVEMENTS WERE FOUND ON EXTRAPOLATION OF BASE MODELS ON NEW BIGGER RADIUS DATASETS