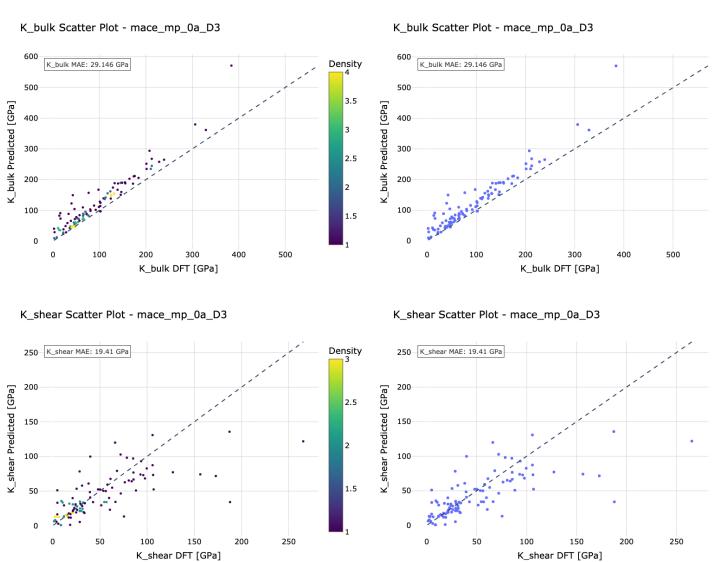
Elasticity Report

Bulk and Shear Moduli MAE Table

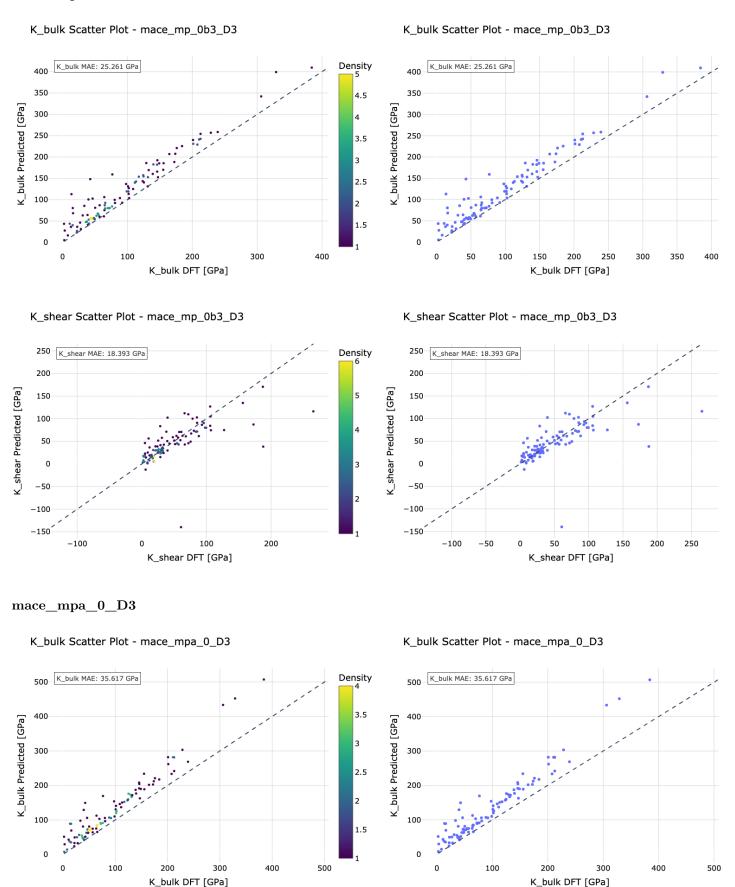
| Model | K_bulk [GPa] | K_shear [GPa] | Elasticity Score \downarrow | Rank |
|-------------------------------|--------------|---------------|-------------------------------|------|
| mace_mp_0a_D3 | 29.146 | 19.41 | 1 | 3 |
| $mace_mp_0b3_D3$ | 25.261 | 18.393 | 0.907 | 2 |
| $mace_mpa_0_D3$ | 35.617 | 20.019 | 1.127 | 4 |
| $mace_omat_0_D3$ | 34.017 | 22.04 | 1.151 | 5 |
| $mace_matpes_PBE_0_D3$ | 18.974 | 15.751 | 0.731 | 1 |
| $mace_matpes_r2scan_0_D3$ | 35.829 | 21.172 | 1.16 | 6 |

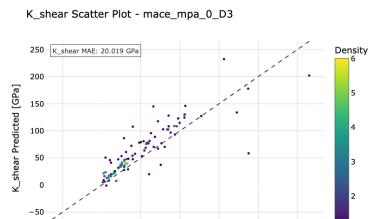
Scatter and density Plots

 $mace_mp_0a_D3$



$mace_mp_0b3_D3$



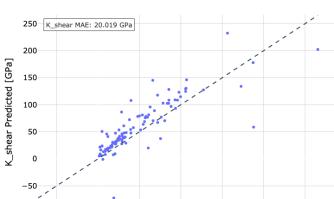


100

K_shear DFT [GPa]

200

250



100

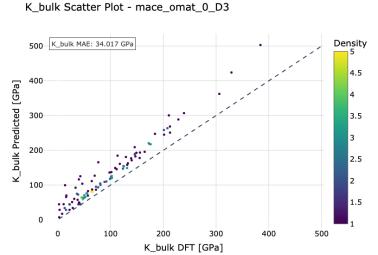
K_shear DFT [GPa]

200

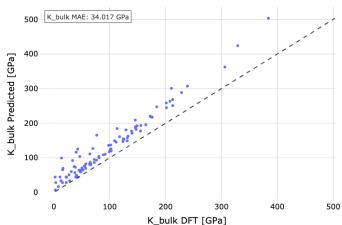
250

K_shear Scatter Plot - mace_mpa_0_D3

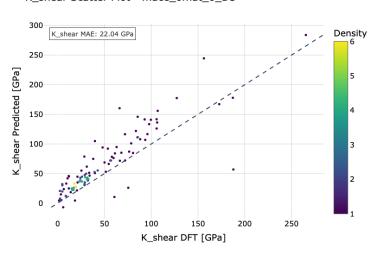
 $mace_omat_0_D3$



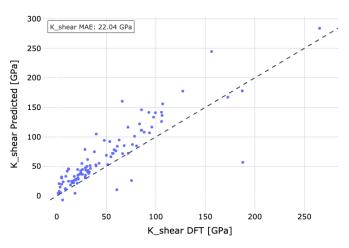
K_bulk Scatter Plot - mace_omat_0_D3



K_shear Scatter Plot - mace_omat_0_D3



K_shear Scatter Plot - mace_omat_0_D3



$mace_matpes_PBE_0_D3$

K_bulk Scatter Plot - mace_matpes_PBE_0_D3 K_bulk Scatter Plot - mace_matpes_PBE_0_D3 450 K_bulk MAE: 18.974 GPa 450 K_bulk MAE: 18.974 GPa Density 3.5 K_bulk Predicted [GPa] K_bulk Predicted [GPa] 1.5 K_bulk DFT [GPa] K_bulk DFT [GPa] K_shear Scatter Plot - mace_matpes_PBE_0_D3 K_shear Scatter Plot - mace_matpes_PBE_0_D3 K_shear MAE: 15.751 GPa Density 6 K_shear MAE: 15.751 GPa K_shear Predicted [GPa] K_shear Predicted [GPa] K_shear DFT [GPa] K_shear DFT [GPa]

 $mace_matpes_r2scan_0_D3$

