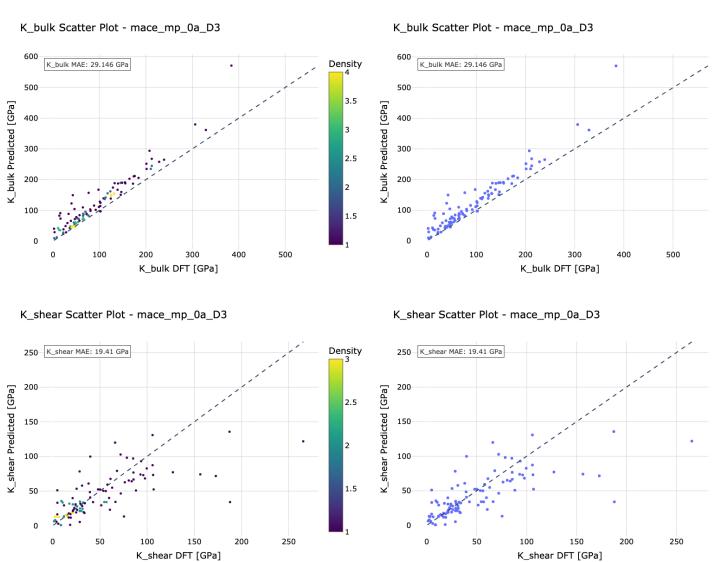
# **Elasticity Report**

### Bulk and Shear Moduli MAE Table

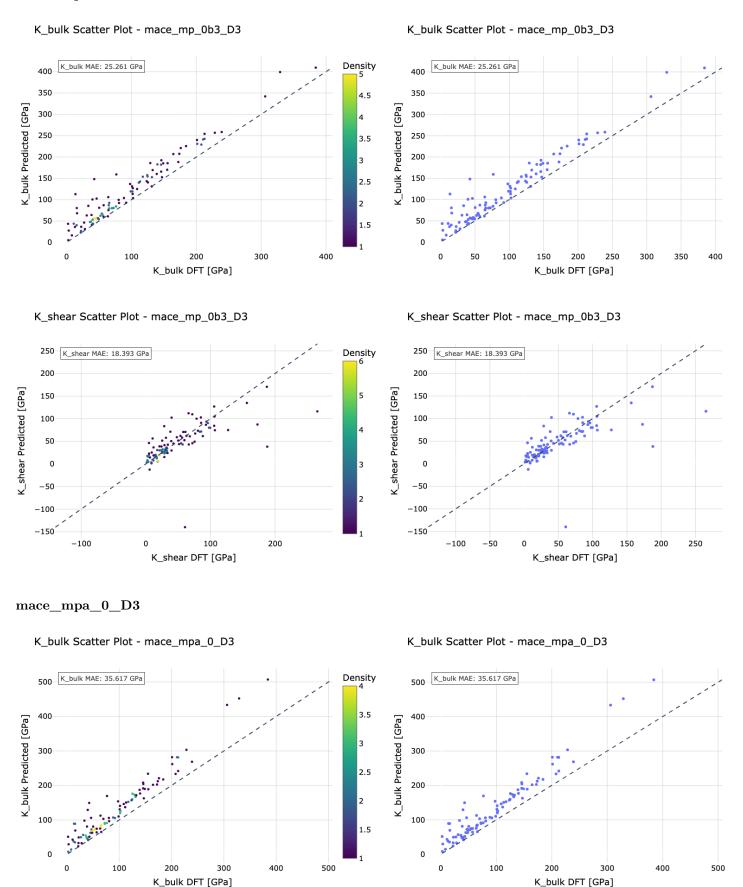
Model	K_bulk [GPa]	K_shear [GPa]	Elasticity Score $\downarrow$	Rank
mace_mp_0a_D3	29.146	19.41	1	3
$mace_mp_0b3_D3$	25.261	18.393	0.907	2
$mace\_mpa\_0\_D3$	35.617	20.019	1.127	4
$mace\_omat\_0\_D3$	34.017	22.04	1.151	5
$mace\_matpes\_PBE\_0\_D3$	18.974	15.751	0.731	1
$mace\_matpes\_r2scan\_0\_D3$	35.829	21.172	1.16	6

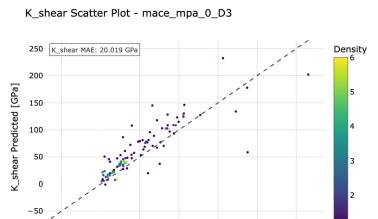
## Scatter and density Plots

 $mace\_mp\_0a\_D3$ 



#### $mace_mp_0b3_D3$



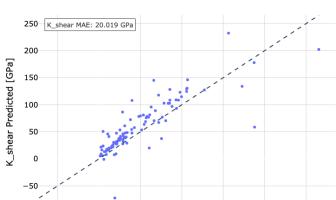


100

K\_shear DFT [GPa]

200

250



100

K\_shear DFT [GPa]

200

250

K\_shear Scatter Plot - mace\_mpa\_0\_D3

 $mace\_omat\_0\_D3$ 

500 K\_bulk MAE: 34.017 GPa

400

400

3.5

4.5

4

200

100

200

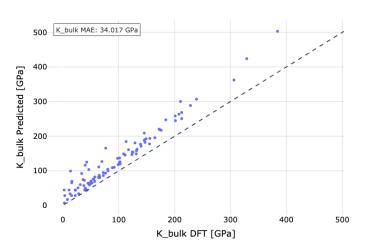
300

400

500

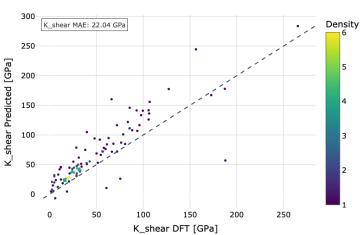
K\_bulk DFT [GPa]

K\_bulk Scatter Plot - mace\_omat\_0\_D3

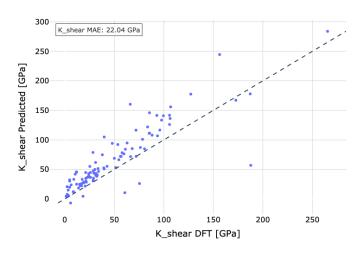


K\_shear Scatter Plot - mace\_omat\_0\_D3

K\_bulk 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]

 $mace\_matpes\_r2scan\_0\_D3$ 

