# **Elasticity Report**

# Bulk and Shear Moduli MAE Table

Model	K_bulk [GPa]	K_shear [GPa]	Elasticity Score (avg)	Rank
mace_mp_0a_D3	48.032	13.867	30.95	4
$mace\_mp\_0b3\_D3$	56.672	23.4	40.036	6
$mace\_mpa\_0\_D3$	41.211	3.442	22.326	3
$mace\_omat\_0\_D3$	22.798	11.507	17.152	2
$mace\_matpes\_PBE\_0\_D3$	47.555	16.274	31.914	5
$mace\_matpes\_r2scan\_0\_D3$	30.493	3.101	16.797	1

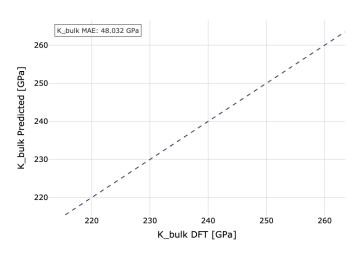
# Scatter and density Plots

 $mace\_mp\_0a\_D3$ 

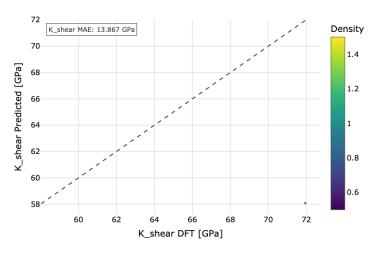
K\_bulk Scatter Plot - mace\_mp\_0a\_D3

K\_bulk MAE: 48.032 GPa Density K\_bulk Predicted [GPa] 250 1.2 240 0.8 230 0.6 220 220 230 240 250 260 K\_bulk DFT [GPa]

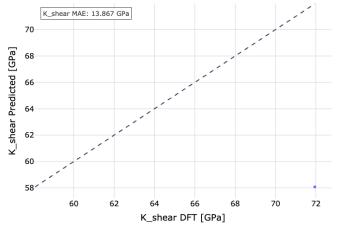
K\_bulk Scatter Plot - mace\_mp\_0a\_D3



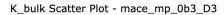
K\_shear Scatter Plot - mace\_mp\_0a\_D3



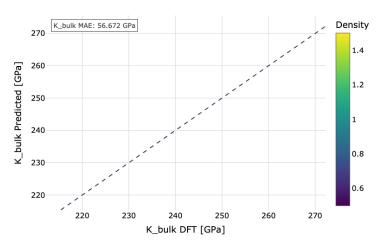
K\_shear Scatter Plot - mace\_mp\_0a\_D3

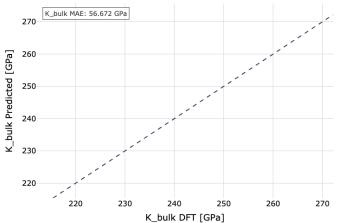


# $mace\_mp\_0b3\_D3$



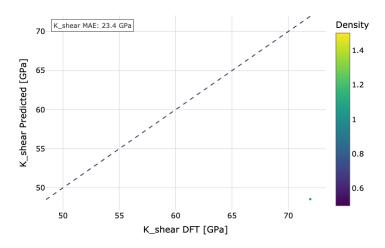
# K\_bulk Scatter Plot - mace\_mp\_0b3\_D3

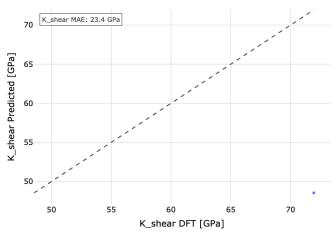




K\_shear Scatter Plot - mace\_mp\_0b3\_D3

K\_shear Scatter Plot - mace\_mp\_0b3\_D3

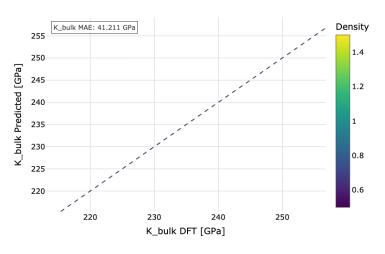


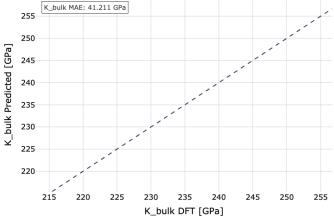


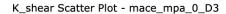
 $mace\_mpa\_0\_D3$ 

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

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



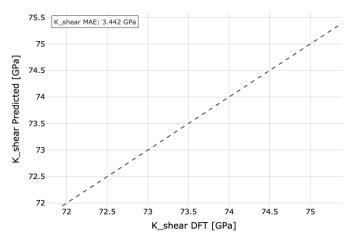




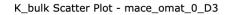
# 75.5 K\_shear MAE: 3.442 GPa 75 1.4 1.2 1.2 73.5 72 72 72.5 73 73.5 74 74.5 75 0.6

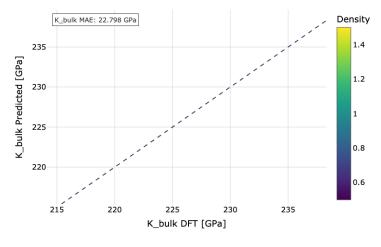
K\_shear DFT [GPa]

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

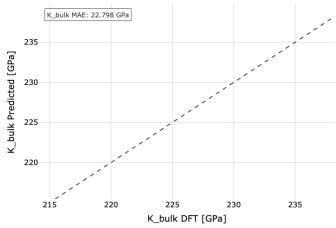


# $mace\_omat\_0\_D3$

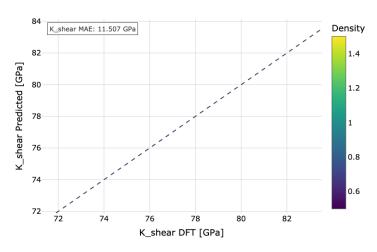




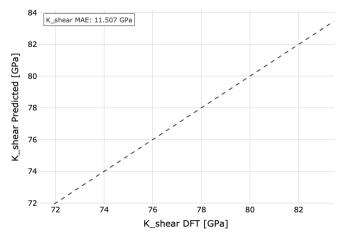
### K\_bulk Scatter Plot - mace\_omat\_0\_D3



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

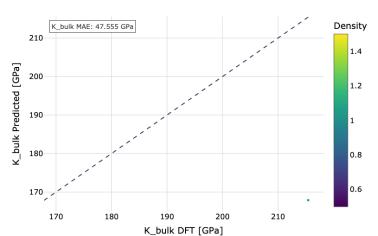


## K\_shear Scatter Plot - mace\_omat\_0\_D3

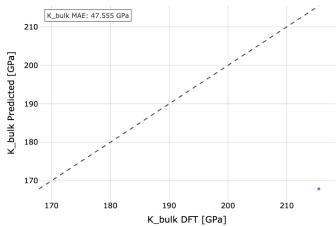


### $mace\_matpes\_PBE\_0\_D3$

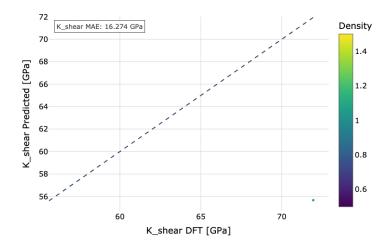
K\_bulk Scatter Plot - mace\_matpes\_PBE\_0\_D3



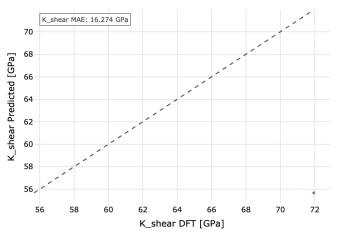
K\_bulk Scatter Plot - mace\_matpes\_PBE\_0\_D3



K\_shear Scatter Plot - mace\_matpes\_PBE\_0\_D3

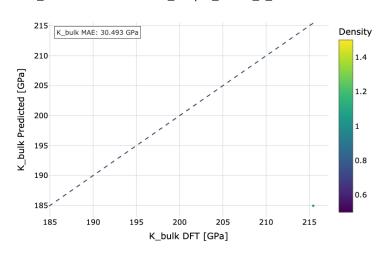


K\_shear Scatter Plot - mace\_matpes\_PBE\_0\_D3

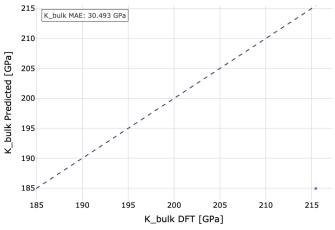


 $mace_matpes_r2scan_0_D3$ 

K\_bulk Scatter Plot - mace\_matpes\_r2scan\_0\_D3



K\_bulk Scatter Plot - mace\_matpes\_r2scan\_0\_D3



# K\_shear Scatter Plot - mace\_matpes\_r2scan\_0\_D3

# K\_shear Scatter Plot - mace\_matpes\_r2scan\_0\_D3

