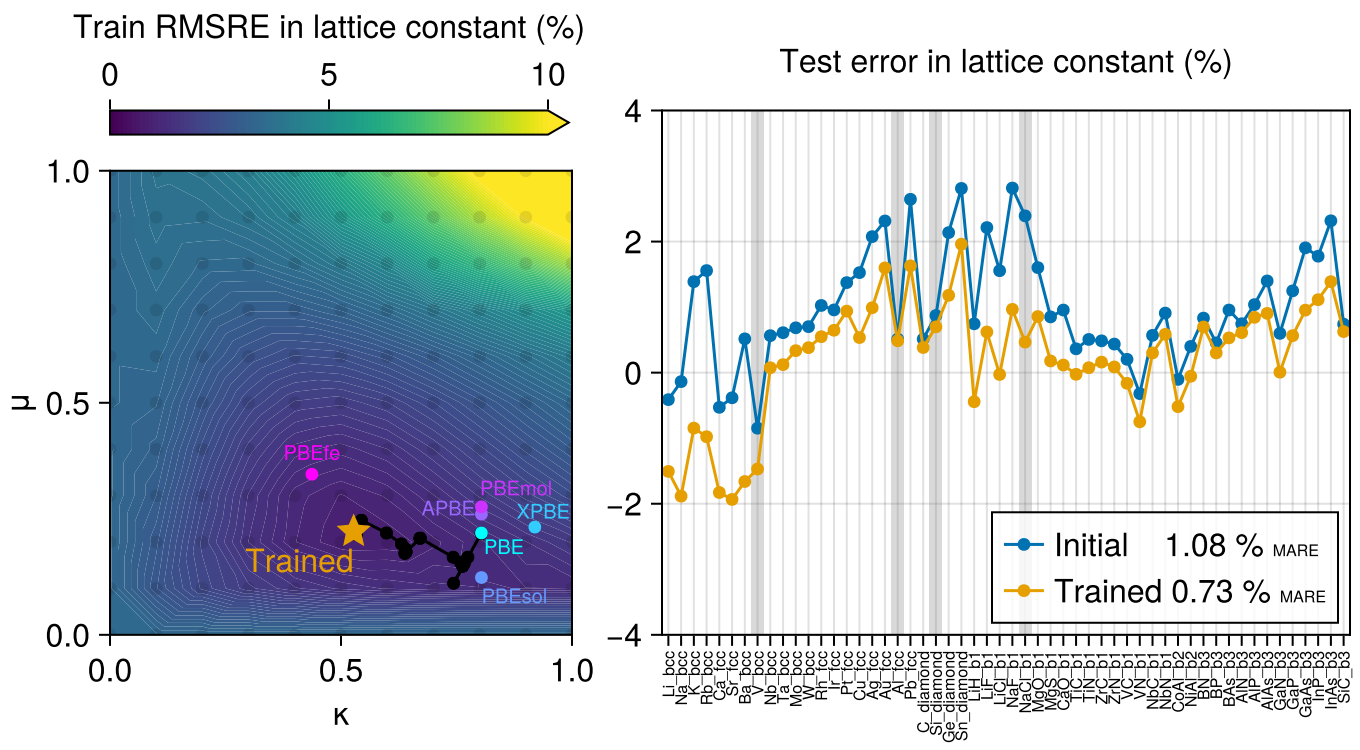
Train RMSRE in lattice constant (%)
0
5
10
1.0
0.5
0.0
μ
0.0
0.5
1.0
κ
PBEfe
PBEmol
APBE
XPBE
PBE
PBEsol
Trained
Test error in lattice constant (%)
4
2
0
−2
−4
Initial 1.08 % MARE
Trained 0.73 % MARE
Li_bcc
Na_bcc
K_bcc
Rb_bcc
Ca_fcc
Sr_fcc
Ba_bcc
V_bcc
Nb_bcc
Ta_bcc
Mo_bcc
W_bcc
Rh_fcc
Ir_fcc
Pt_fcc
Cu_fcc
Ag_fcc
Au_fcc
Al_fcc
Pb_fcc
C_diamond
Si_diamond
Ge_diamond
Sn_diamond
LiH_b1
LiF_b1
LiCl_b1
NaF_b1
NaCl_b1
MgO_b1
MgS_b1
CaO_b1
TiN_b1
ZrC_b1
ZrN_b1
VC_b1
VN_b1
NbC_b1
NbN_b1
CoAl_b2
NiAl_b2
BP_b3
BN_b3
BAs_b3
AlN_b3
AlP_b3
AlAs_b3
GaN_b3
GaP_b3
GaAs_b3
InP_b3
InAs_b3
SiC_b3