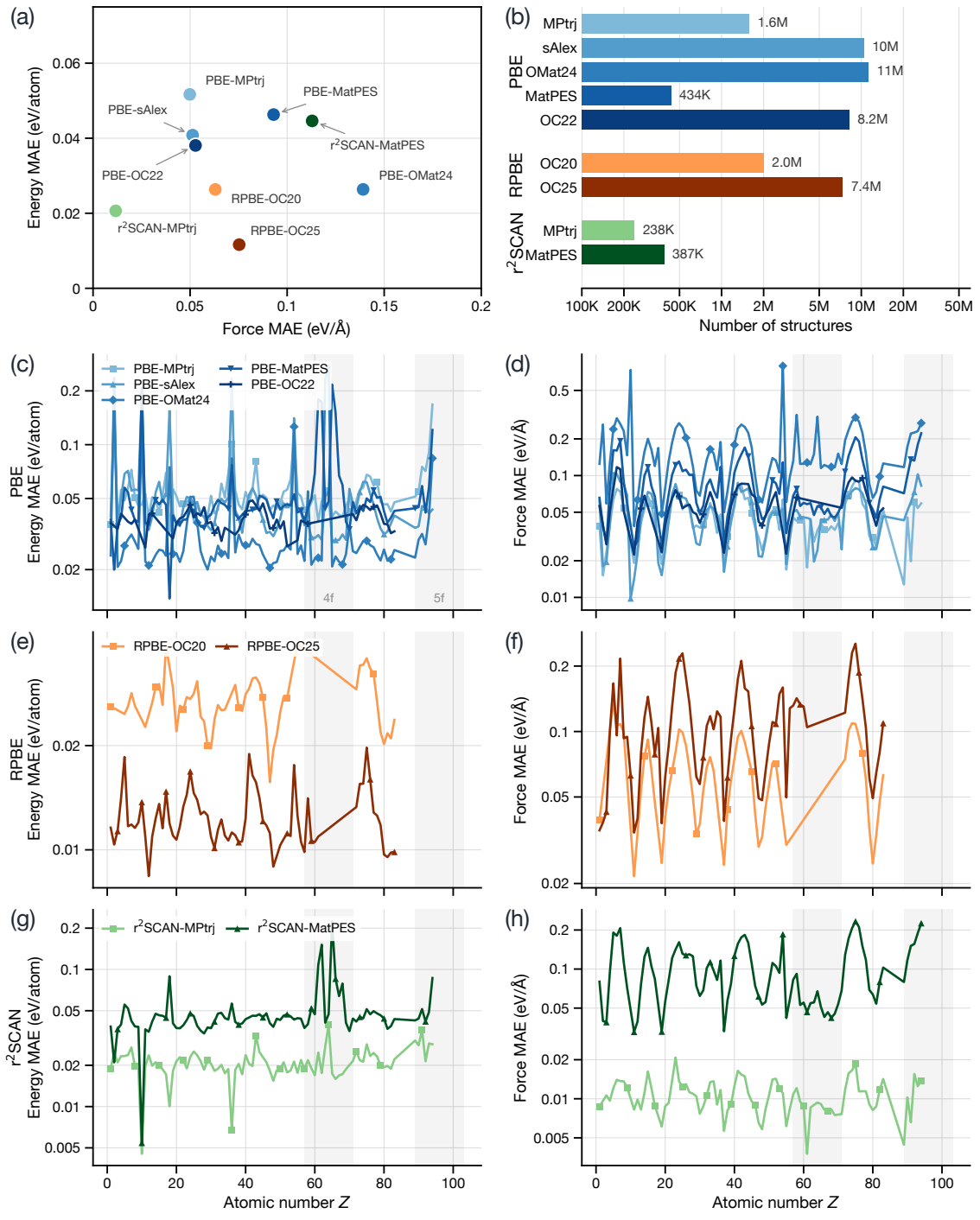

(a)
Energy MAE (eV/atom)
Force MAE (eV/Å)
PBE-MPtrj
PBE-MatPES
PBE-sAlex
r²SCAN-MatPES
PBE-OC22
PBE-OMat24
RPBE-OC20
r²SCAN-MPtrj
RPBE-OC25
(b)
PBE
RPBE
r²SCAN
MPtrj
sAlex
OMat24
MatPES
OC22
OC20
OC25
1.6M
10M
11M
434K
8.2M
2.0M
7.4M
238K
387K
Number of structures
(c)
PBE
Energy MAE (eV/atom)
PBE-MPtrj
PBE-sAlex
PBE-OMat24
PBE-MatPES
PBE-OC22
4f
5f
(d)
Force MAE (eV/Å)
(e)
RPBE
Energy MAE (eV/atom)
RPBE-OC20
RPBE-OC25
(f)
Force MAE (eV/Å)
(g)
r²SCAN
Energy MAE (eV/atom)
r²SCAN-MPtrj
r²SCAN-MatPES
Atomic number Z
(h)
Force MAE (eV/Å)
Atomic number Z