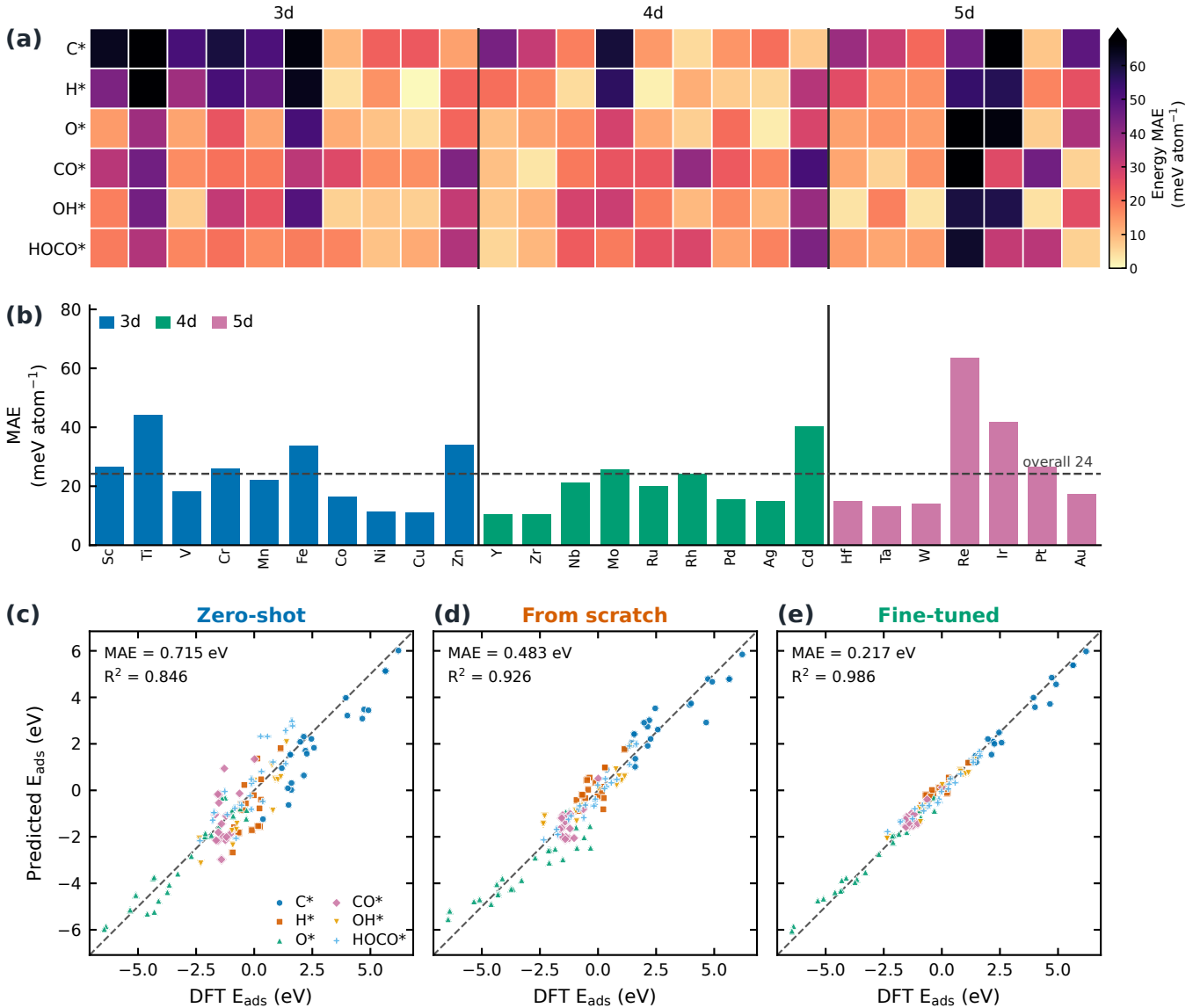

(a)
3d
4d
5d
C*
H*
O*
CO*
OH*
HOCO*
Energy MAE (meV atom^{-1})
0
10
20
30
40
50
60
(b)
3d
4d
5d
MAE (meV atom^{-1})
overall 24
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Y
Zr
Nb
Mo
Ru
Rh
Pd
Ag
Cd
Hf
Ta
W
Re
Ir
Pt
Au
(c)
Zero-shot
MAE = 0.715 eV
R^2 = 0.846
(d)
From scratch
MAE = 0.483 eV
R^2 = 0.926
(e)
Fine-tuned
MAE = 0.217 eV
R^2 = 0.986
Predicted E_{ads} (eV)
DFT E_{ads} (eV)
C*
H*
O*
CO*
OH*
HOCO*