Supplementary information: Convergence and machine learning predictions of Monkhorst-Pack k-points and plane-wave cut-off in high-throughput DFT calculations

Kamal Choudhary, Francesca Tavazza

Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

Table S1: PAW potentials used during the generation of DFT database.

Element	VASP PAW-potential used
Ac	Ac
Ag	Ag
Al	Al
Ar	Ar
As	As
Au	Au
B	B
Ba	Ba_sv
Be	Be_sv
Bi	Bi
Br	Br
C	C
Ca	Ca_sv
Cd	Cd
Ce	Ce
Cl	Cl
Co	Co
Cr	Cr_pv
Cs	Cs_sv

Cu	Cu_pv
Dy	Dy_3
Er	Er_3
Eu	Eu
F	F
Fe	Fe_pv
Ga	Ga_d
Gd	Gd
Ge	Ge_d
H	H
He	He
Hf	Hf_pv
Hg	Hg
Ho	Ho_3
I	I
In	In_d
Ir	Ir
K	K_sv
Kr	Kr
La	La
Li	Li_sv
Lu	Lu_3
Mg	Mg_pv

Mn	Mn_pv
Mo	Mo_pv
N	N
Na	Na_pv
Nb	Nb_pv
Nd	Nd_3
Ne	Ne
Ni	Ni_pv
Np	Np
O	O
Os	Os_pv
P	P
Pa	Pa
Pb	Pb_d
Pd	Pd
Pm	Pm_3
Pr	Pr_3
Pt	Pt
Pu	Pu
Rb	Rb_sv
Re	Re_pv
Rh	Rh_pv
Ru	Ru_pv

S	S
Sb	Sb
Sc	Sc_sv
Se	Se
Si	Si
Sm	Sm_3
Sn	Sn_d
Sr	Sr_sv
Ta	Ta_pv
Tb	Tb_3
Tc	Tc_pv
Te	Te
Th	Th
Ti	Ti_pv
Tl	Tl_d
Tm	Tm_3
U	U
V	V_pv
W	W_pv
Xe	Xe
Y	Y_sv
Yb	Yb_2
Zn	Zn

Zr	Zr_sv

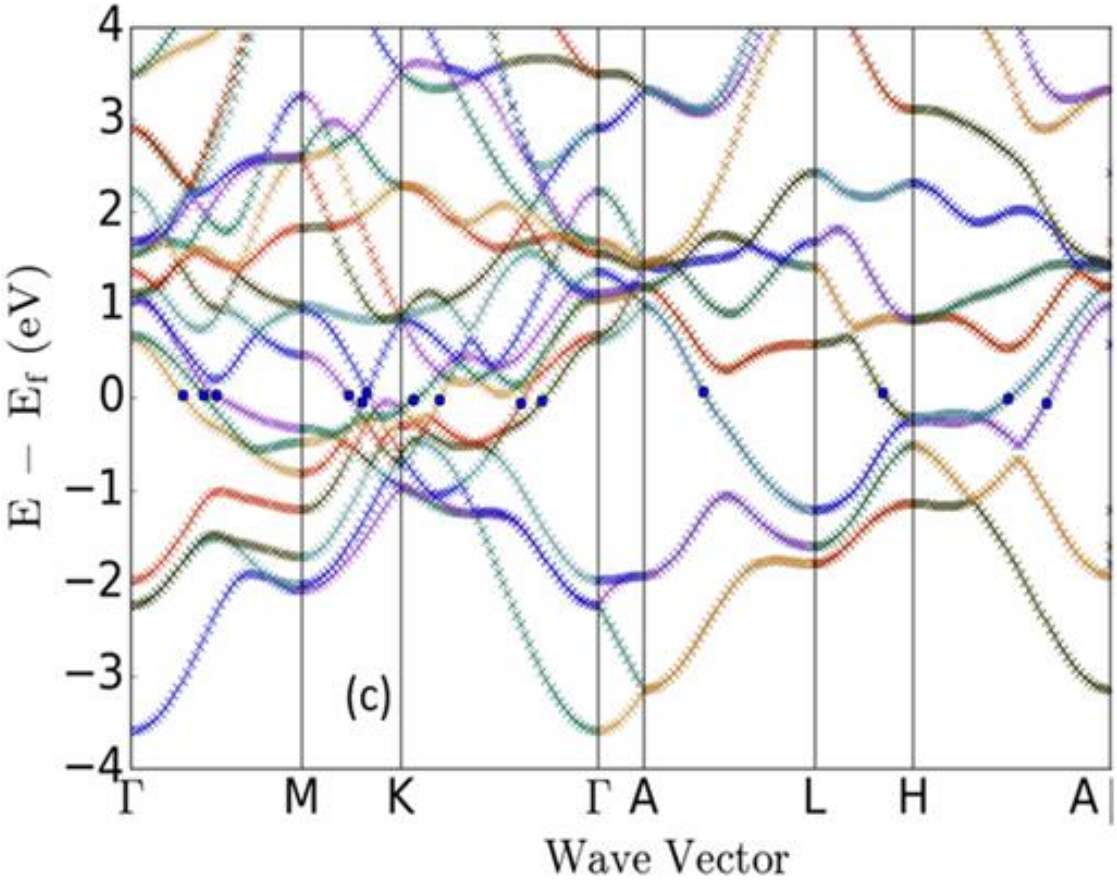

Fig. S1 An example is shown for band-crossings in Pr (JVASP-14689). The dots represent the bands crossing the Fermi-level.

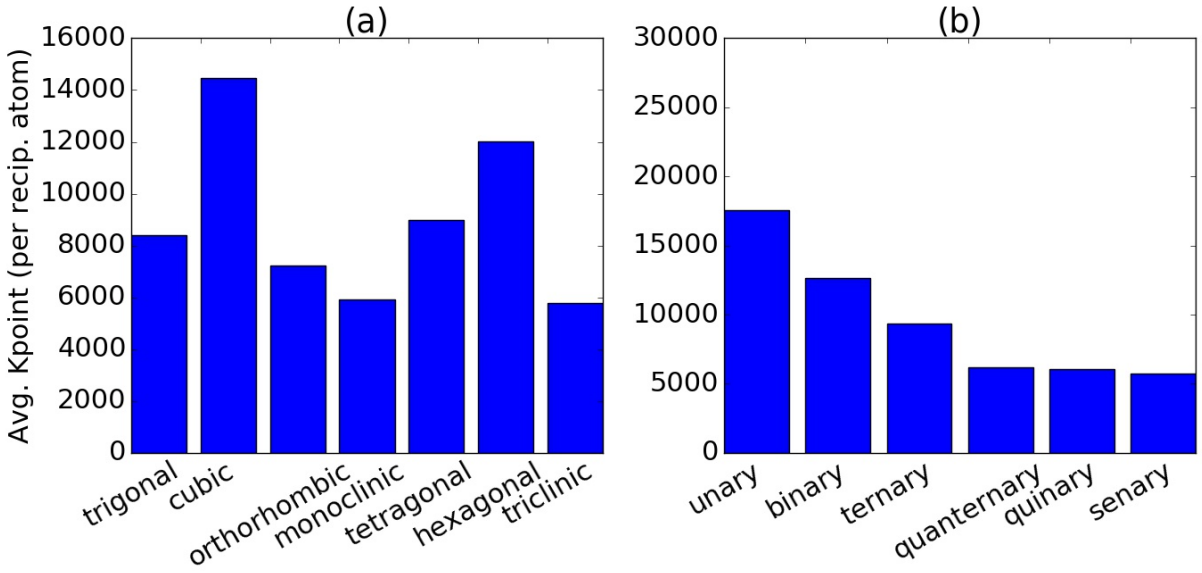

Fig. S2 Correlation of density based average k-points for the seven crystal systems and number of atoms in the cell.