Supplementary Materials

Convolutional Neural Networks for Crystal Material Property Prediction Using Hybrid Orbital-Field Matrix and Magpie Descriptors

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Electron configuration

Table S1: Electron configuration of atoms using in data set[1]

Z	Element name	Non-zero element(s) of one-hot-vector	Atomic electron configuration
1	H	s^1	$1s^1$
5	B	s^2,p^1	$[He]2s^22p^1$
6	C	s^2,p^2	$[He]2s^22p^2$
7	N	s^2,p^3	$[He]2s^22p^3$
8	O	s^2,p^4	$[He]2s^22p^4$
16	S	s^2,p^4	$[Ne]3s^23p^4$
21	Sc	s^2,d^1	$[Ar]4s^23d^1$
22	Ti	s^2,d^2	$[Ar]4s^23d^2$
13	V	s^2,d^3	$[Ar]4s^23d^3$
14	Cr	s^1,d^5	$[Ar]4s^13d^5$
15	MN	s^2,d^5	$[Ar]4s^23d^5$
16	Fe	s^2,d^6	$[Ar]4s^23d^6$
17	Co	s^2,d^7	$[Ar]4s^23d^7$
18	Ni	s^2,d^8	$[Ar]4s^23d^8$
19	Cu	s^1,d^{10}	$[Ar]4s^13d^{10}$
30	Zn	s^2,d^{10}	$[Ar]4s^23d^{10}$
39	Y	s^2,d^1	$[Kr]5s^24d^1$
40	Zr	s^2,d^2	$[Kr]5s^24d^2$
41	Nb	s^1,d^4	$[Kr]5s^14d^4$
42	Mo	s^1,d^5	$[Kr]5s^14d^5$
43	Tc	s^2,d^5	$[Kr]5s^24d^5$
44	Ru	s^1,d^7	$[Kr]5s^14d^7$
45	Rh	s^1,d^8	$[Kr]5s^14d^8$
46	Pd	s^{10}	$[Kr]4s^{10}$
47	Ag	s^1,d^{10}	$[Kr]5s^14d^{10}$
48	Cd	s^2,d^{10}	$[Kr]5s^24d^{10}$
57	La	s^2,d^1	$[Xe]6s^25d^1$
58	Ce	s^2,d^1,f^1	$[Xe]6s^25d^14f^1$
59	Pr	s^2,f^3	$[Xe]6s^24f^3$
60	Nd	s^2,f^4	$[Xe]6s^24f^4$
61	Pm	s^2,f^5	$[Xe]6s^24f^5$
62	Sm	s^2,f^6	$[Xe]6s^24f^6$
63	Eu	s^2,f^7	$[Xe]6s^24f^7$
64	Gd	s^2,d^1,f^7	$[Xe]6s^25d^14f^7$
65	Tb	s^2,f^9	$[Xe]6s^24f^9$
66	Dy	s^2,f^{10}	$[Xe]6s^24f^{10}$
67	Ho	s^2,f^{11}	$[Xe]6s^24f^{11}$

68	Er	s^2,f^{12}	$[Xe]6s^24f^{12}$
69	Tm	s^2,f^{13}	$[Xe]6s^24f^{13}$
70	Yb	s^2,f^{14}	$[Xe]6s^24f^{14}$
71	Lu	s^2,d^1,f^{14}	$[Xe]6s^25d^14f^{14}$
72	Hf	s^2,d^2,f^{14}	$[Xe]6s^25d^24f^{14}$
73	Ta	s^2,d^3,f^{14}	$[Xe]6s^25d^34f^{14}$
74	W	s^2,d^4,f^{14}	$[Xe]6s^25d^44f^{14}$
75	Re	s^2,d^5,f^{14}	$[Xe]6s^25d^54f^{14}$
76	Os	s^2,d^6,f^{14}	$[Xe]6s^25d^64f^{14}$
77	Ir	s^2,d^7,f^{14}	$[Xe]6s^25d^74f^{14}$
78	Pt	s^1,d^9,f^{14}	$[Xe]6s^15d^94f^{14}$
79	Au	s^1,d^{10},f^{14}	$[Xe]6s^15d^{10}4f^{14}$

[1] Tien L P, Kino H, Terakura K, Miyake T, Tsuda K, Takigawa I, Hieu C D. SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS, 2017, 18(1):756-765.

Architectures of CNN for OFM descriptor and Magpie descriptor

Table S2: Architectures of CNN for OFM descriptor

Layer	Filter size	# of filters or elements
Convolution	5*5	32
ReLU	-	-
Convolution	3*3	32
ReLU	-	-
Max pooling	2*2	-
Convolution	3*3	64
ReLU	-	-
Fully connected	-	48
ReLU	-	-
Fully connected	-	32
ReLU	-	-
Fully connected	-	1

Table S3: Architectures of CNN for Magpie descriptor

Layer	Filter size	# of filters or elements
Convolution	3*3	32
ReLU	-	-
Convolution	3*3	48
ReLU	-	-
Max pooling	2*2	-
Convolution	3*3	64
ReLU	-	-
Fully connected	-	48
ReLU	-	-
Fully connected	-	32
ReLU	-	-
Fully connected	-	1

Figures of DFT result and predict result

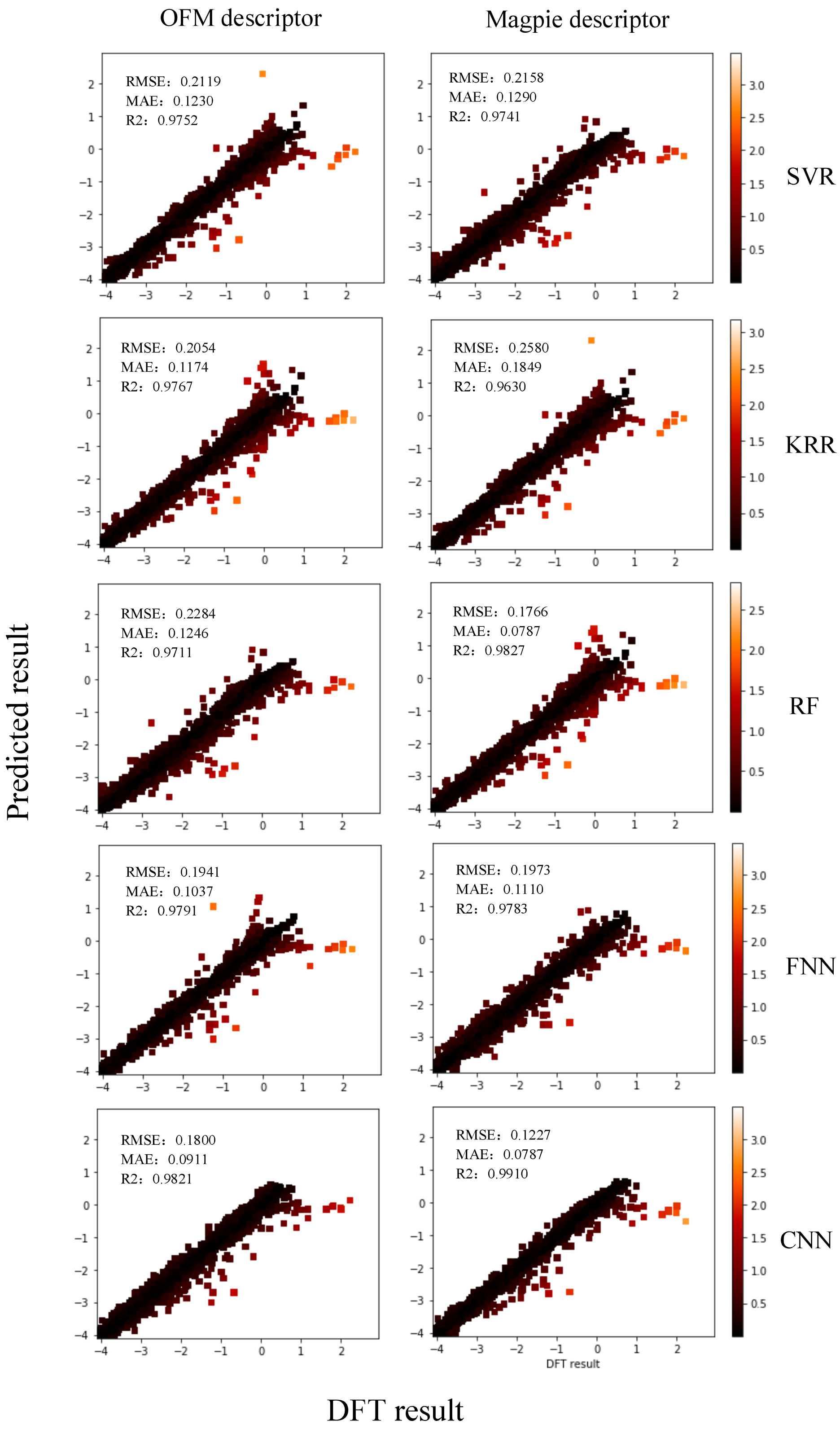

Figure S1: Scatter plots and error metrics for CNN and several regression method, the color of the points indicates the bias between DFT result and predicted result