

Supplemental Information for

Machine learning bandgaps of double perovskites

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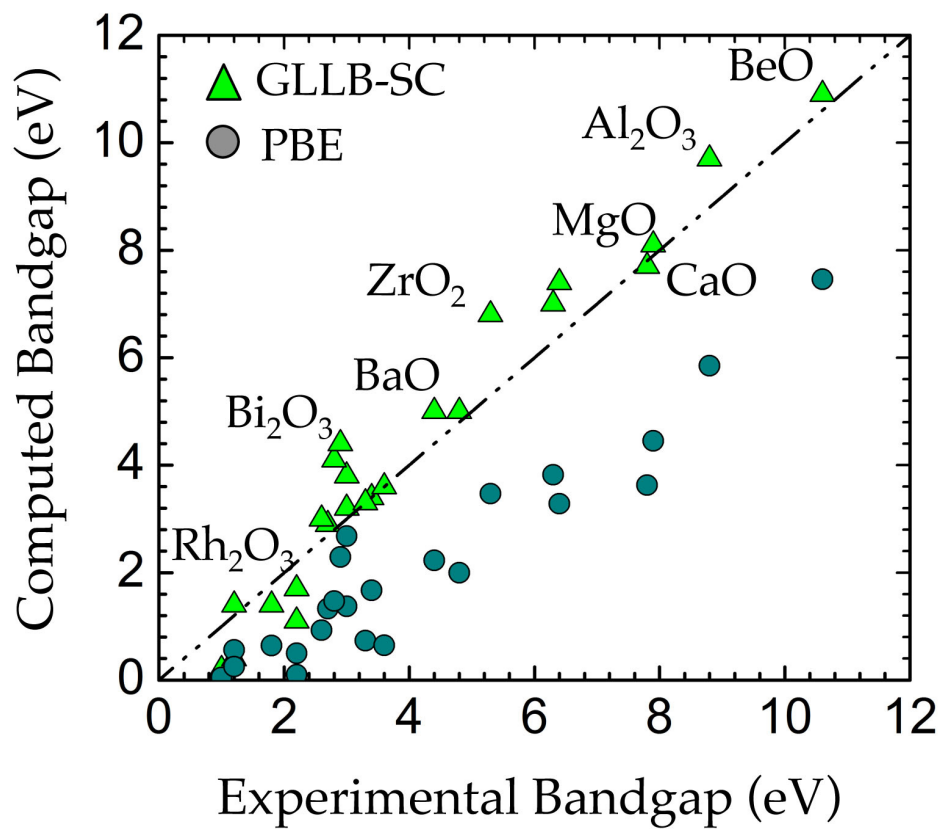


Table 1. Identified optimal primary Ω -D descriptors.

Primary features and optimal primary Ω -D descriptors			
Down-selected primary features		Identities of the primary descriptors	
Primary feature	Feature representation	Descriptor dimension	Descriptor representation
f_1	r_{dA}^+	1-D	$[f_2]$
f_2	l_A^+	2-D	$[f_2, f_{13}]$
f_3	h_A^+	3-D	$[f_2, f_9, f_{13}]$
f_4	χ_A^-	4-D	$[f_2, f_5, f_9, f_{12}]$
f_5	χ_B^+	5-D	$[f_2, f_5, f_9, f_{12}, f_{13}]$
f_6	r_{dA}^-	6-D	$[f_2, f_3, f_5, f_9, f_{12}, f_{13}]$
f_7	l_B^-	7-D	$[f_2, f_3, f_5, f_7, f_9, f_{12}, f_{13}]$
f_8	r_{dB}^+	8-D	$[f_2, f_3, f_5, f_7, f_9, f_{12}, f_{13}, f_{15}]$
f_9	χ_B^-	9-D	$[f_2, f_3, f_4, f_5, f_7, f_9, f_{12}, f_{13}, f_{15}]$
f_{10}	r_{dB}^-	10-D	$[f_2, f_3, f_4, f_5, f_7, f_9, f_{12}, f_{13}, f_{15}, f_{16}]$
f_{11}	l_B^+	11-D	$[f_1, f_2, f_3, f_4, f_5, f_7, f_9, f_{12}, f_{13}, f_{15}, f_{16}]$
f_{12}	l_A^-	12-D	$[f_1, f_2, f_3, f_4, f_5, f_7, f_9, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}]$
f_{13}	h_B^+	13-D	$[f_1, f_2, f_3, f_4, f_5, f_7, f_9, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}]$
f_{14}	h_A^-	14-D	$[f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_9, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}]$
f_{15}	h_B^-	15-D	$[f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_9, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}]$
f_{16}	r_{sA}^-	16-D	$[f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8, f_9, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}]$

Table 2. Identified optimal compound Ω -D descriptors.

Compound features and optimal compound Ω -D descriptors			
Down-selected compound features		Identities of the compound descriptors	
Compound feature	Feature representation	Descriptor dimension	Descriptor representation
f_1	$(r_{sA}^+)^2 \cdot (I_A^+)^3 \cdot \sqrt{(I_A^+)}$	1-D	[f_1]
f_2	$(r_{sA}^+)^2 \cdot (I_A^+)^3 \cdot \exp(\chi_B^-)$	2-D	[f_2, f_{15}]
f_3	$(h_A^+)^2 \cdot (r_{pB}^+)^3 \cdot \exp(I_B^-)$	3-D	[f_2, f_3, f_{15}]
f_4	$(I_A^+)^3 \cdot (I_A^+)^3 \cdot \exp(r_{pB}^+)$	4-D	[f_2, f_3, f_{11}, f_{15}]
f_5	$(r_{pB}^+)^3 \cdot \sqrt{(h_A^+)} \cdot \exp(I_B^-)$	5-D	[$f_1, f_3, f_9, f_{12}, f_{15}$]
f_6	$(r_{dA}^+)^3 \cdot \exp(r_{pB}^-) \cdot \exp(I_A^-)$	6-D	[$f_1, f_3, f_6, f_8, f_{12}, f_{15}$]
f_7	$(\chi_A^+)^3 \cdot \exp(r_{dB}^+) \cdot \exp(I_A^-)$	7-D	[$f_1, f_2, f_3, f_6, f_8, f_{12}, f_{15}$]
f_8	$\sqrt{(h_A^-)} \cdot \ln(1 + \chi_A^-) \cdot \ln(1 + I_A^-)$	8-D	[$f_1, f_2, f_3, f_6, f_8, f_{11}, f_{12}, f_{15}$]
f_9	$(h_B^+)^2 \cdot (\chi_A^+)^3 \cdot \ln(1 + I_A^-)$	9-D	[$f_1, f_2, f_3, f_6, f_8, f_{10}, f_{11}, f_{12}, f_{15}$]
f_{10}	$(I_A^+)^3 \cdot (I_A^+)^3 \cdot \ln(1 + I_A^-)$	10-D	[$f_1, f_2, f_3, f_6, f_8, f_{11}, f_{12}, f_{13}, f_{15}, f_{16}$]
f_{11}	$(\chi_A^+)^3 \cdot \sqrt{(I_A^-)} \cdot \exp(h_B^-)$	11-D	[$f_1, f_2, f_3, f_6, f_8, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]
f_{12}	$(r_{dB}^+)^3 \cdot (h_B^+)^3 \cdot (I_B^-)^3$	12-D	[$f_1, f_2, f_3, f_6, f_8, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]
f_{13}	$\sqrt{(\chi_A^+)} \cdot \sqrt{(h_B^+)} \cdot \sqrt{(r_{sA}^+)}$	13-D	[$f_1, f_2, f_3, f_6, f_7, f_8, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]
f_{14}	$(I_A^+)^2 \cdot (r_{pB}^+)^3 \cdot \exp(I_B^-)$	14-D	[$f_1, f_2, f_3, f_6, f_7, f_8, f_9, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]
f_{15}	$(\chi_B^+)^2 \cdot \sqrt{(\chi_A^+)} \cdot \sqrt{(L_B^+)}$	15-D	[$f_1, f_2, f_3, f_5, f_6, f_7, f_8, f_9, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]
f_{16}	$(r_{dB}^+)^2 \cdot \sqrt{(I_A^-)} \cdot \exp(L_B^-)$	16-D	[$f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8, f_9, f_{10}, f_{11}, f_{12}, f_{13}, f_{14}, f_{15}, f_{16}$]

References

1. Castelli, I.E., Olsen, T., Datta, S., Landis, D.D., Dahl, S., Thygesen, K.S., Jacobsen, K.W. Energy Environ. Sci. 5, 5814 (2012).