

## Electronic Supporting Information

### **Accelerating the Exploration of Novel Perovskite-Structured Metal Borohydrides with Enhanced Dehydrogenation Performance Through Machine Learning**

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Table S1 Coordination number and oxidation state of metal ions in perovskite structured metal borohydrides.

Structure Type	perovskite structure		Double perovskite structure		
	A-site	B-site	A-site	B <sub>1</sub> -site	B <sub>2</sub> -site
Metal Position	A-site	B-site	A-site	B <sub>1</sub> -site	B <sub>2</sub> -site
Coordination Number	12	6	12	6	6
Oxidation State	+1	+2	+1	+1	+3

Table S2 Physical and chemical properties of elements

Number	Property Name	Explanation	Abbreviation
1	Density	-	D
2	at. wt	Relative Atomic Mass	Wt
3	BCC-energy	Energy in BCC Database	BCC-e
4	BCC-fermi	Fermi Energy	BCC-fermi
5	BCC-volume	Volume in BCC Database	BCC-v
6	GS-energy	Energy in GS Database	GS-e
7	ICSD-Volume	Volume in ICSD Database	ICSD-V
8	Covalent radius	-	Cov-R
9	Ionization Energy	-	IE
10	Atomic Radius	-	AtoR
11	Electron Affinity	-	EA
12	At. Radius	Ionic Radius	At. R
13	Atomic Volume	-	AtoV
14	1st Ionization Potential	-	1stIP
15	2nd Ionization Potential	-	2ndIP
16	3rd Ionization Potential	-	3rdIP
17	Coefficient of Thermal Expansion	-	COTE
18	Specific heat capacity	-	SHC
19	Thermal conductivity	-	TC
20	Heat of fusion	-	HoF
21	Heat of Vaporization	-	HoV
22	At.	Atomic Number	At.
23	Melting	Melting Point	Melting
24	Boiling	Boiling Point	Boiling
25	Electronegativity	Pauling Electronegativity	Ele

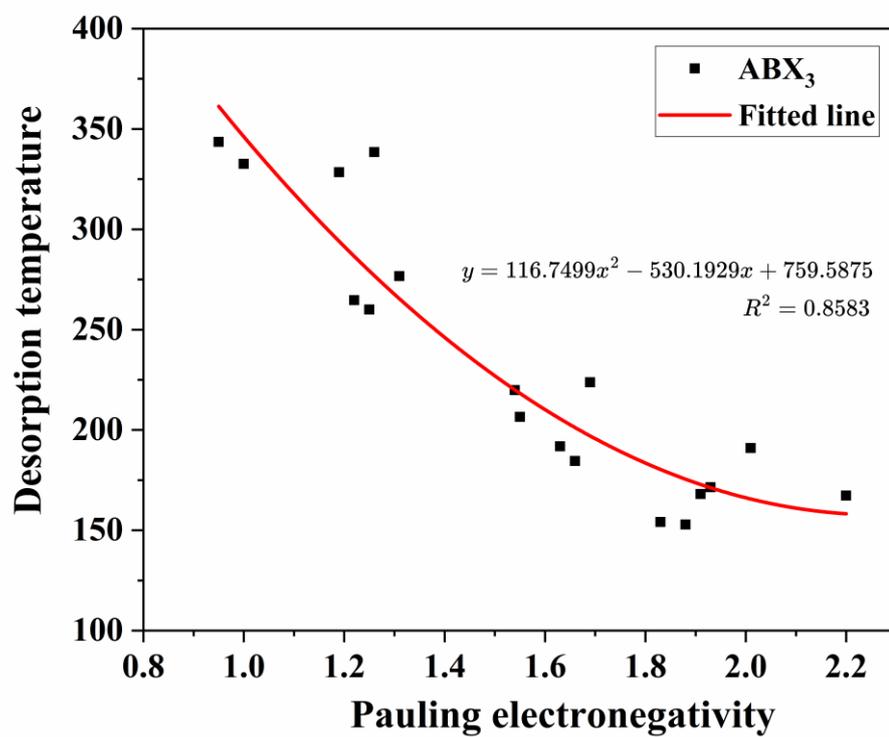


Fig. S1 Relationship between the hydrogen desorption temperature and the electronegativity of the B-site metal cations in single perovskite metal borohydrides.

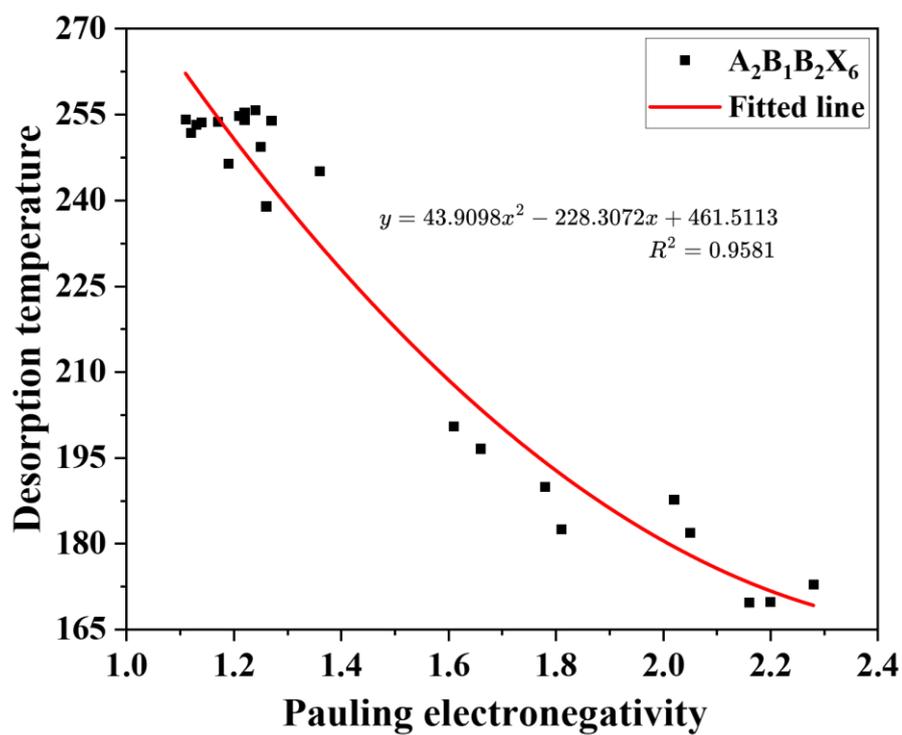


Fig. S2 Relationship between the hydrogen desorption temperature and the electronegativity of the B2-site metal cations in double perovskite metal borohydrides.