Supplementary Information

Generative Design of Stable Semiconductor Materials Using Deep Learning and Density Functional Theory

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Supplementary Note 1: The Elemental and Electronic Properties for Feature Engineering

In addition to the crystal symmetry of the materials, the following atomic and electronic properties were considered to develop the deep neural network model. Here, BCC indicates body-centered cubic, and FCC means face-centered cubic.

Atomic volume	Is Mendeleev	Column number
Atomic number	Is meta	Covalent radius
Atomic weight	Is nonmetal	Density
BCC energy diff	Is metalloid	First ionization energy
BCC effective lattice constant	Is alkali	Ground state band gap
BCC fermi	Is d-block	Ground state efflatcnt
BCC magnetic moment	Is f-block	Ground state estBCClatcnt
BCC volume padiff	Number of valence	Ground state estFCClatcnt
BCC volume pa.	Number of unfilled	Ground state magnetic moment
Boiling temperature	Number of s valance	Ground state volume pa
ICSD volume	Space group number	Row number
Number of d unfilled	Number of d valence	Number of f unfilled
Number of f valence	Number of p unfilled	Number of p valence
Number of s unfilled	Oxidation states	Polarizability

Supplementary Note 2: The classification report of random forest classifier

Supplementary Table 1: The classification report of the test set for the non-metal/metal random forest classifier trained with all the quaternary materials.

	Precision	Recall	F1-score	Support
Metal	0.77	0.62	0.69	197
Non-metal	0.88	0.94	0.91	584
Accuracy			0.86	781
Macro Avg	0.83	0.78	0.80	781
Weighted Avg	0.85	0.86	0.85	781

Supplementary Note 3: Information of Existing $AA'MH_6$ Semiconductors

The following information was taken from the open quantum materials database (OQMD) [1], the Material Project (MP) database [2], and the results from Kadir et al. [3]. OQMD contain the data of only $NaCaIrH_6$, $NaSrIrH_6$, and $NaBaIrH_6$ semiconductors.

Supplementary Table 2: The lattice parameter (a) and bond lengths in Å, and the formation energies in eV/atom for $AA'MH_6$ materials in OQMD.

Material	a	A-H	M-H	A-M	A-A′	E_{form}
$NaCaIrH_6$	5.01321	2.50819	1.68341	3.06995	3.54487	-0.657
$NaSrIrH_6$	5.18736	2.59794	1.68534	3.17659	3.66802	-0.620
$NaBaIrH_6$	5.44633	2.73337	1.68961	3.33518	3.85114	-0.526

Supplementary Table 3: The bandgaps in eV for $AA'MH_6$ semiconductors published in OQMD (E_g^a), MP database (E_g^b) and Kadir et al. (E_g^c).

Material	E_g^a (eV)	E_g^b (eV)	E_g^c (eV)
$NaCaIrH_6$	3.5	3.53	3.33
$NaSrIrH_6$	3.5	3.38	3.21
$NaBaIrH_6$	3.2	-	3.09
$KBaIrH_6$	-	-	3.01
$KBaIrH_6$	-	-	2.91

Supplementary Note 4: Comparing Bandgaps calculated using the PBE and HSE06 methods

Supplementary Table 4: Bandgaps calculated based on PBE and HSE06 methods in eV.

Material	E_g-PBE	E_g-HSE06
$BaNaRhH_6$	3.02	4.34
$BaSrZnH_6$	1.59	2.59
$BaCsAlH_6$	2.94	3.88
$SrTlIrH_6$	1.62	2.51
$CsKSiH_6$	2.164	3.15
$KNaNiH_6$	3.30	4.23
$NaYRuH_6$	2.53	4.06
$CaScMnH_6$	1.27	3.04
$NaZrMnH_6$	1.57	3.34
$AgZrMnH_6$	1.41	3.07

Supplementary Note 5: Predicted Semiconductors

The following table contains the chemical formulas of the semiconductors predicted by the RFC model. The structures of those materials can be downloaded from the Carolina Materials database at `http://www.carolinamatdb.org/`.

Supplementary Table 5: The semiconductors predicted by the RFC model

$AlGaH_6Os$	$CsBaNiH_6$	$KInH_6Pt$	$LiMgH_6Ir$	$RbHgAsH_6$	$SrYH_6Rh$	Cs_6H_6IrPt
$BaAlTlH_6$	$CsHgAsH_6$	$KLiH_6Pt$	$LiScH_6Os$	$RbScTcH_6$	$YCdCoH_6$	Cs_6ReH_6Au
$BaCaH_6Ir$	$CsKSiH_6$	$KNaCuH_6$	$LiYFeH_6$	$RbTlH_6Pd$	$YCoAgH_6$	Cs_6ReSnH_6
$BaCaH_6Rh$	$CsRbH_6Pb$	$KNaH_6Pt$	$LiYH_6Ir$	$RbYMgH_6$	$YCoH_6Pb$	Cs_6SiH_6Rh
$BaCrH_6Ru$	$CsRbSnH_6$	$KNaNiH_6$	$LiZrCrH_6$	$ScCoAgH_6$	$YCrInH_6$	Cs_6SnH_6Ir
$BaMgZnH_6$	$CsSrCoH_6$	$KRbCuH_6$	$MgCdCoH_6$	$ScMnGeH_6$	$YMnHgH_6$	Cs_6SnH_6W
$BaMnVH_6$	$CsSrGaH_6$	$KRbGeH_6$	$MgGaH_6Ir$	$ScMnSnH_6$	$YMnZnH_6$	Cs_6TlH_6Os
$BaNaH_6Rh$	$CsSrInH_6$	$KRbSnH_6$	Na_6AlGaH	$ScMnZnH_6$	$YScCrH_6$	Cs_6VSiH_6
$BaNaNiH_6$	$CsZnSbH_6$	$KScAlH_6$	Na_6CaTlH	$SrBeTcH_6$	$YScFeH_6$	$CsSc_6TcTe_6$
$BaScH_6Os$	$HfMnCdH_6$	$KScZnH_6$	Na_6CdInH	$SrCaH_6Rh$	$YZnH_6Ru$	K_6CoH_6Rh
$BaSrCuH_6$	$HfScBeH_6$	$KTiH_6Os$	Na_6ScBiH	$SrCrReH_6$	$YZrCoH_6$	K_6MnAlH_6
$BaSrMgH_6$	$HfScFeH_6$	$KTlNiH_6$	$NaCaCoH_6$	$SrHgGeH_6$	$YZrCrH_6$	KZr_6Te_6As
$BaSrZnH_6$	$KAlZnH_6$	KVH_6Ru	$NaCaH_6Ir$	$SrHgH_6Pt$	$ZnReH_6Pt$	KZr_6Te_6Rh
$BaZnTcH_6$	$KBaBH_6$	KYH_6Ir	$NaMgH_6Pd$	$SrMgSiH_6$	$ZrFeNiH_6$	Rb_6MgSiH_6
$CaAlH_6Ir$	$KBaH_6Pt$	KYH_6Os	$NaMgH_6Pt$	$SrMnH_6Os$	$ZrMnAgH_6$	Rb_6NiSnH_6
$CaCoAgH_6$	$KBaTiH_6$	KYH_6Pt	$NaScH_6Os$	$SrMnVH_6$	$ZrMnZnH_6$	Sr_6SiTe_6As
$CaScMnH_6$	$KBiH_6Ir$	$KZnAsH_6$	$NaYH_6Ru$	$SrTiMnH_6$	$BaMg_6Te_6Ir$	YSc_6MoH_6
$CaYNiH_6$	$KCaCoH_6$	Li_6FeSiH	$NaZnGaH_6$	$SrTlH_6Ir$	Ca_6MgTe_6Pt	
$CaZrH_6Ir$	$KCaH_6Pt$	Li_6NiGeH	$NaZrMnH_6$	$SrTlNiH_6$	Cs_6AlVH_6	
$CsBaAlH_6$	$KCdSbH_6$	$LiBeH_6Os$	NiH_6PtPb	$SrVCrH_6$	Cs_6GaSiH_6	

Supplementary References

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