Supplemental Information

The Github repository containing the code used to create the models in this paper can be found here: GitHub repository

Predictions for the MXenes in the "Pivotal Role of Surface Terminations in MXene Thermodynamic Stability" dataset can be found in .csv format here: "Pivotal Role of Surface Terminations in MXene Thermodynamic Stability" dataset predictions

Predictions for the MXenes in the aNANt dataset can be found in .csv format here: aNANt dataset predictions

cfid input feature list containing 438 input features (see supplemental information from "Atomistic Line Graph Neural Network for improved materials property predictions" for more information)

Addition ('add'), multiplications ('mult'), subtraction ('subs') and quotient ('divi') of hfus, polzbl, first_ion_en, mol_vol, bp, mp, therm_cond and voro_coord, atom_rad, elec_aff, X, and atom_mass were performed to give additional chemical descriptors.

TABLE I: Details of element based chemical descriptors. Here is a list of the types of input features in the cfid feature set with their corresponding definitions. Addition ('add'), multiplications ('mult'), subtraction ('subs') and quotient ('divi') of hfus, polzbl, first_ion_en, mol_vol, bp, mp, therm_cond and voro_coord, atom_rad, elec_aff, X, and atom_mass were performed to give additional chemical descriptors.

Descriptor_name	**Details**
jv_enp	Energy per atom of an element from JARVIS-DFT
KV	Bulk modulus of an element from JARVIS-DFT
GV	Shear modulus of an element from JARVIS-DFT
C-m	(m=0 to 35) Elastic constants of an element from JARVIS-DFT (total 36)
op_eg	OptB88vdW bandgap during SCF for an element
mop_eg	OptB88vdW bandgap during linear optics for an element
voro_coord	Voronoi coordination number of an elemental-crystal structure
ndunfilled	Number of unfilled d-orbitals
ndvalence	Number of valence d-orbitals
nsunfilled	Number of unfilled s-orbitals
nsunfilled	Number of valence s-orbitals
npunfilled	Number of unfilled p-orbitals
npvalence	Number of valence p-orbitals
nfunfilled	Number of unfilled f-orbitals
nfvalence	Number of valence f-orbitals
first_ion	First ionization energy of an element
oq_bg	OQMD bandgap for an element
elec_aff	Electron affinity
vol_pa	Volume per atom of an element
hfus	Heat of fusion of an element
oq_enp	OQMD energy per atom
Polariz	Polarizability
Z	Atomic number
X	Electronegativity
row	Row number in the periodic table
column	Column number in the periodic table
max_oxid_s	Maximum oxidation state
min_oxid_s	Minimum oxidation state
block	s,p,d,f block assigned to 0,1,2,3 blocks
is_alkali	Is it alkali element 0/1
is_alkaline	Is it alkaline element 0/1
is_metalloid	Is it metalloid element 0/1
is_noble_gas	Is it noble gas element 0/1
is_transition_metal	Is it transition element 0/1
is_metalloid	Is it metalloid element 0/1
is_halogen	Is it halogen element 0/1
is_lanthanoid	Is it lanthanoid element 0/1
is_actinoid	Is it actinoid element 0/1
atom_mass	Atomic mass
atom_rad	Atomic radii
therm_cond	Thermal conductivity
mol_vol	Molar volume
bp	Boiling point
mp	Melting point
avg_ion_rad	Average ionic radii
polzbl	Polarizability
e1	Static dielectric function in x-direction from JARVIS-DFT using OptB88vdW functional
e2	Static dielectric function in y-direction from JARVIS-DFT using OptB88vdW functional
e3	Static dielectric function in z-direction from JARVIS-DFT using OptB88vdW functional
me1	Static dielectric function in x-direction from JARVIS-DFT using TB-mBJ potential
me2	Static dielectric function in y-direction from JARVIS-DFT using TB-mBJ potential
me3	Static dielectric function in z-direction from JARVIS-DFT using TB-mBJ potential

atom_mass
atom_mass_add_atom_rad
atom_mass_add_therm_cond
atom_mass_add_voro_coord
atom_mass_add_X
atom_mass_divi_atom_rad
atom_mass_divi_bp
atom_mass_divi_first_ion_en
atom_mass_divi_hfus
atom_mass_divi_mol_vol
atom_mass_divi_mp
atom_mass_divi_polzbl
atom_mass_divi_therm_cond
atom_mass_divi_voro_coord
atom_mass_mult_atom_rad
atom_mass_mult_therm_cond
atom_mass_mult_voro_coord
atom_mass_mult_X
atom_mass_subs_atom_rad
atom_mass_subs_bp
atom_mass_subs_elec_aff
atom_mass_subs_first_ion_en
atom_mass_subs_hfus
atom_mass_subs_mol_vol
atom_mass_subs_mp
atom_mass_subs_polzbl
atom_mass_subs_therm_cond
atom_mass_subs_voro_coord
atom_mass_subs_X
atom_rad
atom_rad_add_therm_cond
atom_rad_add_voro_coord
atom_rad_add_X
atom_rad_divi_atom_mass
atom_rad_divi_bp
atom_rad_divi_first_ion_en
atom_rad_divi_hfus
atom_rad_divi_mol_vol
atom_rad_divi_mp
atom_rad_divi_polzbl
atom_rad_divi_therm_cond
atom_rad_divi_voro_coord
atom_rad_mult_therm_cond
atom_rad_mult_voro_coord
atom_rad_mult_X
atom_rad_subs_atom_mass
atom_rad_subs_bp
atom_rad_subs_elec_aff
atom_rad_subs_first_ion_en
atom_rad_subs_hfus
atom_rad_subs_mol_vol
atom_rad_subs_mp
atom_rad_subs_polzbl
atom_rad_subs_therm_cond
atom_rad_subs_voro_coord
atom_rad_subs_X
avg_ion_rad
block
bp
bp_add_atom_mass
bp_add_atom_rad
bp_add_mp
bp_add_therm_cond
bp_add_voro_coord
bp_add_X
bp_divi_atom_mass
bp_divi_atom_rad
bp_divi_first_ion_en
bp_divi_hfus
bp_divi_mol_vol
bp_divi_mp
bp_divi_polzbl
bp_divi_therm_cond
bp_divi_voro_coord
bp_mult_atom_mass
bp_mult_atom_rad
bp_mult_mp
bp_mult_therm_cond
bp_mult_voro_coord
bp_mult_X
bp_subs_atom_mass
bp_subs_atom_rad
bp_subs_elec_aff
bp_subs_first_ion_en
bp_subs_hfus
bp_subs_mol_vol
bp_subs_mp
bp_subs_polzbl
bp_subs_therm_cond
bp_subs_voro_coord
bp_subs_X
C-0
C-1
C-10
C-11
C-12
C-13
C-14
C-15
C-16
C-17
C-18
C-19
C-2
C-20
C-21
C-22
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C-25
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C-27

C-28
C-29
C-3
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C-31
C-32
C-33
C-34
C-35
C-4
C-5
C-6
C-7
C-8
C-9
coulmn
e1
e2
e3
elec_aff
elec_aff_add_atom_mass
elec_aff_add_atom_rad
elec_aff_add_bp
elec_aff_add_mol_vol
elec_aff_add_mp
elec_aff_add_therm_cond
elec_aff_add_voro_coord
elec_aff_add_X
elec_aff_mult_atom_mass
elec_aff_mult_atom_rad
elec_aff_mult_bp
elec_aff_mult_mol_vol
elec_aff_mult_mp
elec_aff_mult_therm_cond
elec_aff_mult_voro_coord
elec_aff_mult_X
elec_aff_subs_atom_mass
elec_aff_subs_atom_rad
elec_aff_subs_bp
elec_aff_subs_first_ion_en
elec_aff_subs_hfus
elec_aff_subs_mol_vol
elec_aff_subs_mp
elec_aff_subs_polzbl
elec_aff_subs_therm_cond
elec_aff_subs_voro_coord
elec_aff_subs_X
first_ion_en
first_ion_en_add_atom_mass
first_ion_en_add_atom_rad
first_ion_en_add_bp
first_ion_en_add_elec_aff
first_ion_en_add_mol_vol
first_ion_en_add_mp
first_ion_en_add_therm_cond
first_ion_en_add_voro_coord
first_ion_en_add_X
first_ion_en_divi_atom_mass
first_ion_en_divi_atom_rad
first_ion_en_divi_bp
first_ion_en_divi_hfus
first_ion_en_divi_mol_vol
first_ion_en_divi_mp
first_ion_en_divi_polzbl
first_ion_en_divi_therm_cond
first_ion_en_divi_voro_coord
first_ion_en_mult_atom_mass
first_ion_en_mult_atom_rad
first_ion_en_mult_bp
first_ion_en_mult_elec_aff
first_ion_en_mult_mol_vol
first_ion_en_mult_mp
first_ion_en_mult_therm_cond
first_ion_en_mult_voro_coord
first_ion_en_mult_X
first_ion_en_subs_atom_mass
first_ion_en_subs_atom_rad
first_ion_en_subs_bp
first_ion_en_subs_elec_aff
first_ion_en_subs_hfus
first_ion_en_subs_mol_vol
first_ion_en_subs_mp
first_ion_en_subs_polzbl
first_ion_en_subs_therm_cond
first_ion_en_subs_voro_coord
first_ion_en_subs_X
GV
hfus
hfus_add_atom_mass
hfus_add_atom_rad
hfus_add_bp
hfus_add_elec_aff
hfus_add_first_ion_en
hfus_add_mol_vol
hfus_add_mp
hfus_add_polzbl
hfus_add_therm_cond
hfus_add_voro_coord
hfus_add_X
hfus_divi_atom_mass
hfus_divi_atom_rad
hfus_divi_bp
hfus_divi_first_ion_en
hfus_divi_mol_vol
hfus_divi_mp
hfus_divi_polzbl
hfus_divi_therm_cond
hfus_divi_voro_coord
hfus_mult_atom_mass
hfus_mult_atom_rad
hfus_mult_bp
hfus_mult_elec_aff

hfus_mult_first_ion_en
hfus_mult_mol_vol
hfus_mult_mp
hfus_mult_polzbl
hfus_mult_therm_cond
hfus_mult_voro_coord
hfus_mult_X
hfus_subs_atom_mass
hfus_subs_atom_rad
hfus_subs_bp
hfus_subs_elec_aff
hfus_subs_first_ion_en
hfus_subs_mol_vol
hfus_subs_mp
hfus_subs_polzbl
hfus_subs_therm_cond
hfus_subs_voro_coord
hfus_subs_X
is_actinoid
is_alkali
is_alkaline
is_halogen
is_lanthanoid
is_metalloid
is_noble_gas
is_transition_metal
jv_enp
KV
max_oxid_s
me1
me2
me3
min_oxid_s
mol_vol
mol_vol_add_atom_mass
mol_vol_add_atom_rad
mol_vol_add_bp
mol_vol_add_mp
mol_vol_add_therm_cond
mol_vol_add_voro_coord
mol_vol_add_X
mol_vol_divi_atom_mass
mol_vol_divi_atom_rad
mol_vol_divi_bp
mol_vol_divi_first_ion_en
mol_vol_divi_hfus
mol_vol_divi_mp
mol_vol_divi_polzbl
mol_vol_divi_therm_cond
mol_vol_divi_voro_coord
mol_vol_mult_atom_mass
mol_vol_mult_atom_rad
mol_vol_mult_bp
mol_vol_mult_mp
mol_vol_mult_therm_cond
mol_vol_mult_voro_coord
mol_vol_mult_X
mol_vol_subs_atom_mass
mol_vol_subs_atom_rad
mol_vol_subs_bp
mol_vol_subs_elec_aff
mol_vol_subs_first_ion_en
mol_vol_subs_hfus
mol_vol_subs_mp
mol_vol_subs_polzbl
mol_vol_subs_therm_cond
mol_vol_subs_voro_coord
mol_vol_subs_X
mop_eg
mp
mp_add_atom_mass
mp_add_atom_rad
mp_add_therm_cond
mp_add_voro_coord
mp_add_X
mp_divi_atom_mass
mp_divi_atom_rad
mp_divi_bp
mp_divi_first_ion_en
mp_divi_hfus
mp_divi_mol_vol
mp_divi_polzbl
mp_divi_therm_cond
mp_divi_voro_coord
mp_mult_atom_mass
mp_mult_atom_rad
mp_mult_therm_cond
mp_mult_voro_coord
mp_mult_X
mp_subs_atom_mass
mp_subs_atom_rad
mp_subs_bp
mp_subs_elec_aff
mp_subs_first_ion_en
mp_subs_hfus
mp_subs_mol_vol
mp_subs_polzbl
mp_subs_therm_cond
mp_subs_voro_coord
mp_subs_X
ndunfill
ndvalence
nfunfill
nfvalence
npunfill
npvalence
nsunfill
nsvalence
op_eg
oq_bg
oq_enp
polzbl

polzbl_add_atom_mass
polzbl_add_atom_rad
polzbl_add_bp
polzbl_add_elec_aff
polzbl_add_first_ion_en
polzbl_add_mol_vol
polzbl_add_mp
polzbl_add_therm_cond
polzbl_add_voro_coord
polzbl_add_X
polzbl_divi_atom_mass
polzbl_divi_atom_rad
polzbl_divi_bp
polzbl_divi_first_ion_en
polzbl_divi_hfus
polzbl_divi_mol_vol
polzbl_divi_mp
polzbl_divi_therm_cond
polzbl_divi_voro_coord
polzbl_mult_atom_mass
polzbl_mult_atom_rad
polzbl_mult_bp
polzbl_mult_elec_aff
polzbl_mult_first_ion_en
polzbl_mult_mol_vol
polzbl_mult_mp
polzbl_mult_therm_cond
polzbl_mult_voro_coord
polzbl_mult_X
polzbl_subs_atom_mass
polzbl_subs_atom_rad
polzbl_subs_bp
polzbl_subs_elec_aff
polzbl_subs_first_ion_en
polzbl_subs_hfus
polzbl_subs_mol_vol
polzbl_subs_mp
polzbl_subs_therm_cond
polzbl_subs_voro_coord
polzbl_subs_X
row
therm_cond
therm_cond_add_voro_coord
therm_cond_add_X
therm_cond_divi_atom_mass
therm_cond_divi_atom_rad
therm_cond_divi_bp
therm_cond_divi_first_ion_en
therm_cond_divi_hfus
therm_cond_divi_mol_vol
therm_cond_divi_mp
therm_cond_divi_polzbl
therm_cond_divi_voro_coord
therm_cond_mult_voro_coord
therm_cond_mult_X
therm_cond_subs_atom_mass
therm_cond_subs_atom_rad
therm_cond_subs_bp
therm_cond_subs_elec_aff
therm_cond_subs_first_ion_en
therm_cond_subs_hfus
therm_cond_subs_mol_vol
therm_cond_subs_mp
therm_cond_subs_polzbl
therm_cond_subs_voro_coord
therm_cond_subs_X
voro_coord
voro_coord_divi_atom_mass
voro_coord_divi_atom_rad
voro_coord_divi_bp
voro_coord_divi_first_ion_en
voro_coord_divi_hfus
voro_coord_divi_mol_vol
voro_coord_divi_mp
voro_coord_divi_polzbl
voro_coord_divi_therm_cond
voro_coord_subs_atom_mass
voro_coord_subs_atom_rad
voro_coord_subs_bp
voro_coord_subs_elec_aff
voro_coord_subs_first_ion_en
voro_coord_subs_hfus
voro_coord_subs_mol_vol
voro_coord_subs_mp
voro_coord_subs_polzbl
voro_coord_subs_therm_cond
voro_coord_subs_X
X
X_add_voro_coord
X_mult_voro_coord
X_subs_atom_mass
X_subs_atom_rad
X_subs_bp
X_subs_elec_aff
X_subs_first_ion_en
X_subs_hfus
X_subs_mol_vol
X_subs_mp
X_subs_polzbl
X_subs_therm_cond
X_subs_voro_coord
Z

CGCNN input features: