Element features

Table S1: 58 element features that are used to calculated compositional descriptors. We provide these feature information via our open-source software XenonPy [1]

Feature ID	Description	Unit	Reference
atomic_number	Atomic number		
atomic_radius	Atomic radius	pm	[2, 3]
atomic_radius_rahm	Atomic radius by Rahm et al.	pm	[4, 5, 3]
atomic_volume	Atomic volume	cm^3/mol	[3]
atomic_weight	Atomic weight		[6, 7, 3]
boiling_point	Boiling temperature	K	[3]
bulk_modulus	Bulk modulus	GPa	[8]
c6_gb	C_6 dispersion coefficient in a.u. (Gould & Bučko)	a.u.	[9, 10, 3]
covalent_radius_cordero	Covalent radius by Cerdero et al.	pm	[11, 3]
covalent_radius_pyykko	Single bond covalent radius by Pyykko et al.	pm	[12, 3]
covalent_radius_pyykko_double	Double bond covalent radius by Pyykko et al.	pm	[13, 3]
covalent_radius_pyykko_triple	Triple bond covalent radius by Pyykko et al.	pm	[14, 3]
covalent_radius_slater	Covalent radius by Slater	pm	[2]
density	Density at 295K	g/cm^3	[3]
dipole_polarizability	Dipole polarizability	a.u,	[15, 3]
electron_negativity	Pauling electronegativity		[16]
electron_affinity	Electron affinity	eV	[17, 18, 3]
en_allen	Allen's scale of electronegativity	eV	[19, 20, 3]
en_ghosh	Ghosh's scale of electronegativity		[21, 3]
en_pauling	Pauling's scale of electronegativity		[17, 3]
first_ion_en	First ionisation energy	eV	[17]
fusion_enthalpy	Enthalpy of fusion for elements at their melting temperatures	kJ/mol	[17]
gs_bandgap	DFT bandgap energy of T=0K ground state	eV	[22, 23]
gs_energy	DFT energy per atom (raw VASP value) of T=0K ground state	eV/atom	[22, 23]
gs_est_bcc_latcnt	Estimated BCC lattice parameter based on the DFT volume of the OQMD ground state for each element		[22, 23]
gs_est_fcc_latcnt	Estimated FCC lattice parameter based on the DFT volume of the OQMD ground state for each element	Å	[22, 23]
gs_mag_moment	DFT magnetic momenet of T=0K ground state		[22, 23]
gs_volume_per	DFT volume per atom of T=0K ground state	$Å^3/atom$	[22, 23]
hhi_p	HerfindahlHirschman Index (HHI) production values		[24]
hhi_r	HerfindahlHirschman Index (HHI) reserves values		[24]
heat_capacity_mass	Specific heat capacity at STP	J/mol-K	[17]
heat_capacity_molar	Molar heat capacity at STP	J/mol-K	[17]
icsd_volume	Volume per atom of ICSD phae at STP		[25, 26, 27]
evaporation_heat	Evaporation heat	kJ/mol	[3]

Table S1 continued

Feature ID	Description	Unit	Reference
heat_of_formation	Heat of formation	kJ/mol	[3]
lattice_constant	Lattice constant	Å	[3]
mendeleev_number	Mendeleev's number		[28, 29, 3]
melting_point	Melting temperature	K	[3]
molar_volume	Molar volume	L/mol	[8]
num_unfilled	Number of unfilled valence orbitals		[16]
num_valance	Number of valence electrons		[16]
num_d_unfilled	Number of unfilled d valence orbitals		[16]
num_d_valence	Number of filled d valence orbitals		[16]
num_f_unfilled	Number of unfilled f valence orbitals		[16]
num_f_valence	Number of filled f valence orbitals		[16]
num_p_unfilled	Number of unfilled p valence orbitals		[16]
num_p_valence	Number of filled p valence orbitals		[16]
num_s_unfilled	Number of unfilled s valence orbitals		[16]
num_s_valence	Number of filled s valence orbitals		[16]
period	Period in periodic table		[3]
specific_heat	Specific heat at 20 °C	J/(g mol)	[3]
thermal_conductivity	Thermal conductivity at 25 °C	W/(m K)	[3]
vdw_radius	Van der Waals radius	pm	[17, 3]
vdw_radius_alvarez	Van der Waals radius according to Alvarez	pm	[30, 3]
vdw_radius_mm3	Van der Waals radius from the MM3 FF	pm	[31, 3]
vdw_radius_uff	Van der Waals radius from the UFF	pm	[32, 3]
sound_velocity	Velocity of sound	m/s	[8]
polarizability	Static average electric dipole polarizability	10^{-24}cm^3	[17]

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