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Supporting materials for

DOI: <https://dx.doi.org/10.30919/esmm5f756>

Machine Learning Prediction for Bandgaps of Inorganic Materials

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Appendix

Table A1. 34 features used in the machine learning models.

Atomic number	Metallic valence
Atomic weight	Number of valence electrons
Period number	Number of s electrons
Group number	Number of p electrons
Family number	Number of d electrons
L quantum number	Number of outer shell electrons
Mendeleev number	First ionization energy (kJ/mol)
Atomic radius (Å)	Polarizability
Covalent radius (Å)	Melting point (K)
Zunger radius (Å)	Boiling point (K)
Ionic radius (Å)	Density (g/mL)
Crystal radius (Å)	Specific heat (J/g•K)
Pauling EN	Heat of fusion (kJ/mol)
Martynov-Batsanov EN	Heat of vaporization (kJ/mol)
Gordy EN	Thermal conductivity (W/m•K)
Mulliken EN	Heat atomization (kJ/mol)
Allen EN	Cohesive energy (eV)
