

Machine-Learning-Driven Design of High-Elastocaloric NiTi-Based Shape Memory Alloys

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Table S1. List of features used in M2 and M3. Pink represents the remaining features after filtering by Pearson correlation coefficient.

Abbreviation	Description
dor	Waber–Cromer's pseudopotential radius [49]
en	Electronegativity (Pauling) [50]
mr	Metallic radius [51]
ar	Atomic radius [52]
aw	Atomic weight (Villars, Daams)
val	Valence
rcov	Radii: covalent
wf	Work function
E0	Energy per atom of T=0K ground state
La	Lattice constants a
Ven	Valence electron number [53]
mc	Modulus compression
An	Atomic number
MN	Mendeleev number
eif	Energy ionization first
dve	Distance valence electron (Schubert)
Ns	NsValence
rsh	Radii ionic (Shannon)
n_ws	Electron density at surface of Wigner–Sietz cell
EN	Type of element
HT _I	Temperature of homogenization treatment
Ht _I	Time of homogenization treatment
W _I	Ways of quenching of homogenization treatment
HT _{II}	Temperature of solution treatment
Ht _{II}	Time of solution treatment
W _{II}	Ways of quenching of solution treatment
HT _{III}	Temperature of aging treatment

Ht_{III}	Time of aging treatment
W_{III}	Ways of quenching of aging treatment

Table S2. Thirteen features after Pearson correlation selection for M1.

Abbreviation	Description
n_ws	Electron density at surface of Wigner–Sietz cell
aven	Average electron number
en	Electronegativity (Alfred-Rochow)
dve	Distance valence electron (Schubert)
Ns	NsValence
ar	Atomic radius
E0	Energy per atom of T=0K
rsh	Radii ionic (Shannon)
GS	GSmagmom
LA	Lattice angle
mc	Modulus compression
La	Lattice constants a
wf	Work function

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