**Machine learning-driven Design of High-elastocaloric NiTi-based Shape Memory Alloys**

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**Supplementary materials**

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[42] |
| en | Electronegativity (Pauling) [43] |
| mr | Metallic radius[44] |
| ar | Atomic Radius[45] |
| 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[46] |
| 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 Elements |
|  | Temperature of Homogenization treatment |
|  | Time of Homogenization treatment |
|  | Ways of quenching of Homogenization treatment |
|  | Temperature of Solution treatment |
|  | Time of Solution treatment |
|  | Ways of quenching of Solution treatment |
|  | Temperature of Aging treatment |
|  | Time of Aging treatment |
|  | Ways of quenching of Aging treatment |

Table S2 13 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 Angles | |
| mc | modulus compression | |
| La | Lattice Constants a | |
| wf | work function | |

Table S SMA designed by M1 with S greater than 90 J/Kg·K-1 in 4 iterations.

|  |  |  |
| --- | --- | --- |
| Alloys (at. %) | \_pred(J/Kg·K-1) | \_exp(J/Kg·K-1) |
| Ni49.5Ti49.5Ga1 | 89.03 | 97.91 |
| Ni49Ti50Ge1 | 89.80 | 93.8 |
| Ni49Ti50.5Si0.5 | 84.63 | 93.78 |
| Ni49.5Ti50Te0.5 | 88.27 | 93.77 |
| Ni49Ti50.5In0.5 | 84.33 | 93.41 |
| Ni48.5Ti51Sb0.5 | 87.56 | 92.77 |
| Ni49Ti50.5Sn0.5 | 84.60 | 92.45 |
| Ni49Ti49Be2 | 91.35 | 91.48 |
| Ni49Ti50.5Sc0.5 | 84.62 | 90.72 |