**Auxiliary properties**

**Red:** Theory and Experiment

**Blue:** Theory

**Green:** Experiment

1. *Chemistry*

* **Stoichiometry:** Percentange of each atomic specie in the material.It is derived from “Chemical formula”.

Example: Chemical formula =Fe3Sn1 🡪 Stoichiometry=Fe0.75Sn0.25

* **Atomic species:** Species of the atoms in this material. It is derived from “Chemical formula”.

Example: Chemical formula =Fe3Sn1 🡪 Atomic species=Fe,Sn

* **Species count:** number of species in the system (e.g., binary = 2, ternary = 3, etc.). It is derived from “Chemical formula”.

Example: Chemical formula =Fe3Sn1 🡪 Species count=2

1. *Crystal*

* **Lattice system:** it is derived from “Space group”

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| Lattice System | Space group |
| TRIC | 1,2 |
| MON | 3-15 |
| ORT | 16-74 |
| TET | 75-142 |
| RHO | 146,148,155,160,161,166,167 |
| HEX | 143-145,147,149-154,156-159, 162-165,168-194 |
| CUB | 195-230 |

* **Unit cell atom count:** Number of atoms in the unit cell (integer number). It is derived from “Chemical formula”, just summing the number of atoms.

Example: Chemical formula =Fe3Sn1 🡪 Unit cell atom count=4

* **Atom volume:** “Unit cell volume”/ ”Unit cell atom count”. Decimal representation [min,max]=[0.00000,1000.00000]

1. *Thermodynamics*

* **Atomic energy:** “Unit cell energy”/ “Unit cell atom count”. Decimal representation [min,max]=[-100.0000000,100.0000000]
* **Atomic formation enthalpy:** “Unit cell formation enthalpy”/“Unit cell atom count”. Decimal representation [min,max]=[-1000.0000000,1000.0000000]