The phase map of chemical systems in the Periodic Number representation

Abstract

The phase map of chemical systems of any order, from binary to high-order systems, can be systematically built by using the Periodic Number (PN) of the constituent elements. In particular, the Mendeleev Periodic Number of the elements expresses clearly the chemical similarity along the groups in the Periodic Table.

Therefore, from unary to higher order systems, the phase map of chemical systems in the PN-representation clearly shows the periodicity of chemical properties, phase stability, structure types and highlights the former and non-former regions. The regions where stable phases can be found but are not yet experimentally reported, are the ones investigated via first-principles crystal structure prediction approaches (CSP).

The neighbour crystal structure similarity concept, employed in the PN-based crystals structure prediction (PNscp), reveals effective in predicting the most likely structure representation a possible phase, not yet reported in the literature, can adopt.

The phase stability is then ascertained based on the three fundamental criteria of phase stability at normal (p,T) conditions:

1. thermodynamic stability: existence of a minimum, local and/or global, in the Gibbs free energy.
2. mechanical stability: the necessary and sufficient conditions of the elastic stability are fulfilled (the Born stability criteria).
3. the dynamical stability: all values of the vibrational frequencies throughout the Brillouin zone are real values.

References

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