Alloy design for additive manufacturing
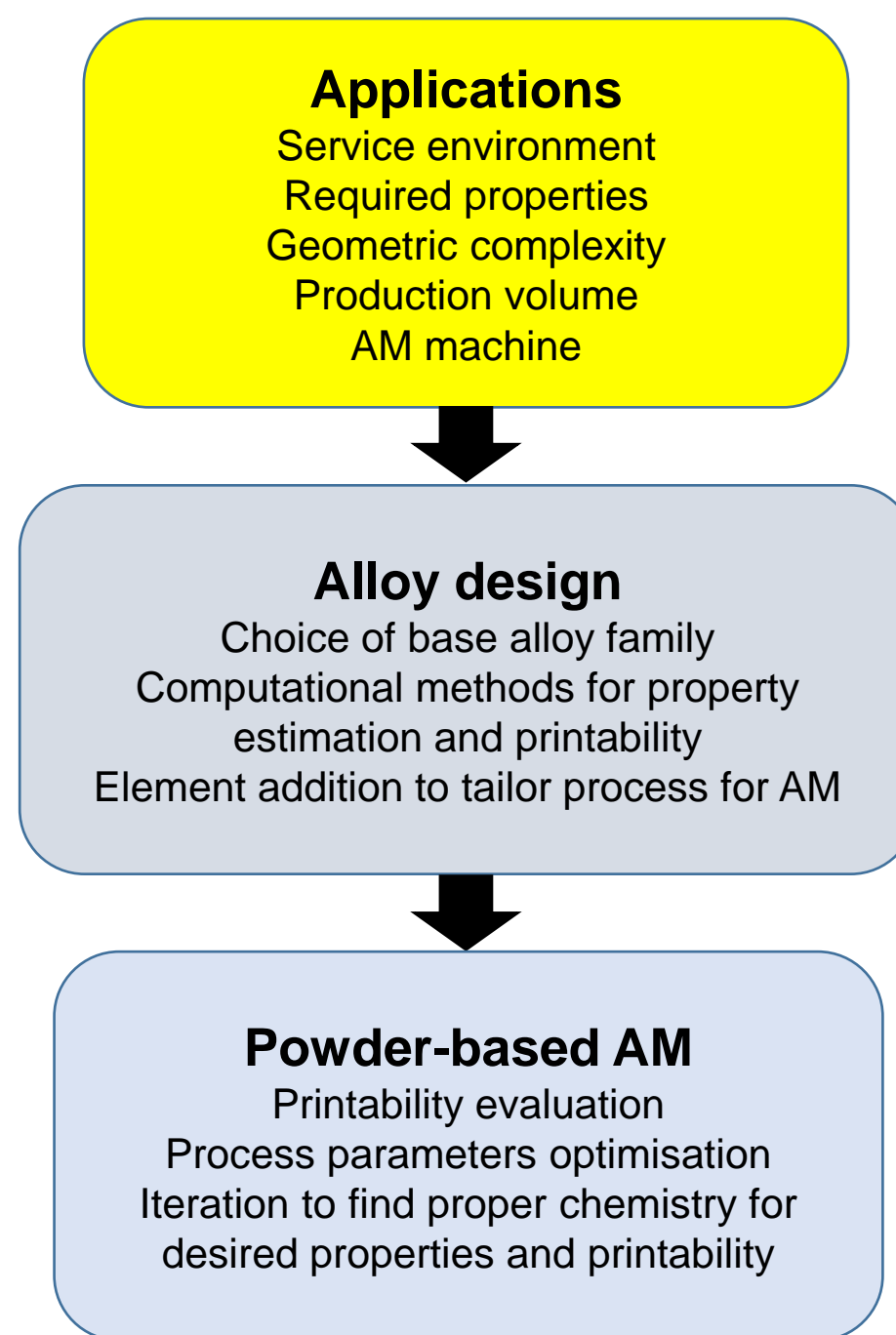
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❑ Summary

Introduction

- Space for alloy discovery
- Complex synergies between processing and properties take place
- Very few material systems have been tailored to additive manufacturing
- Design freedom not yet fully exploited when considering materials

Additive manufacturing-based alloy design

Applications
Service environment
Required properties
Geometric complexity
Production volume
AM machine

Alloy design
Choice of base alloy family
Computational methods for property estimation and printability
Element addition to tailor process for AM

Powder-based AM
Printability evaluation
Process parameters optimisation
Iteration to find proper chemistry for desired properties and printability

Additive manufacturing-based alloy design

Fig. Alloy design for Metal Additive Manufacturing

Source: Zhang et al. 2018 [https://doi.org/10.1002/adem.201700952]

Optimisation methods

3 individuals (each with 4 genes)

0.51	0.33	0.02
0.11	0.64	0.31
0.72	0.99	0.82
0.02	0.62	0.25

Fitness Score: 13% 04% 33%

Start

Generate initial population

Calculate fitness of individuals

Satisfy stop criterion

Yes → End

No →

Roulette selection of parents — Randomly pick parents, weighted by fitness values

Crossover to produce children — Create 2 children by crossing over genes from each parent

Parents:

0.51	0.02
0.11	0.31
0.72	0.82
0.02	0.25

Children:

0.51	0.02
0.11	0.31
0.82	0.72
0.25	0.02

Mutation of children — Ocassionally, randomly mutate one gene

0.48

0.51	0.02
0.11	0.31
0.82	0.72
0.25	0.02

Calculate fitness of children

New generation by "Elitism"

0.51	0.02	0.02
0.48	0.31	0.31
0.82	0.72	0.82
0.25	0.02	0.25

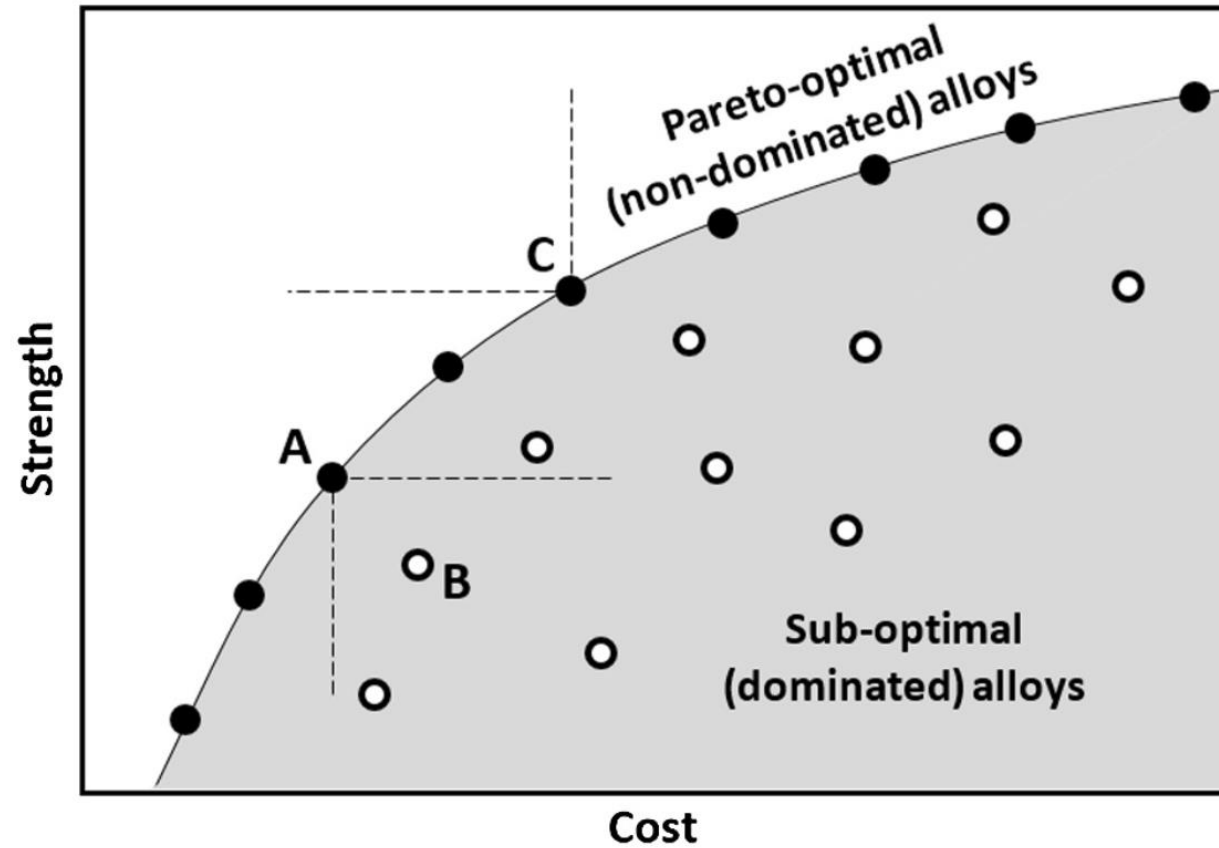**Fig.** Flow diagram of genetic algorithm

Optimisation methods

Fig. Multi-objective optimization (MOO) to maximize the strength and minimize the cost of the alloy

Source: Deschamps et al. 2018 [https://doi.org/10.1016/j.crhy.2018.08.001]
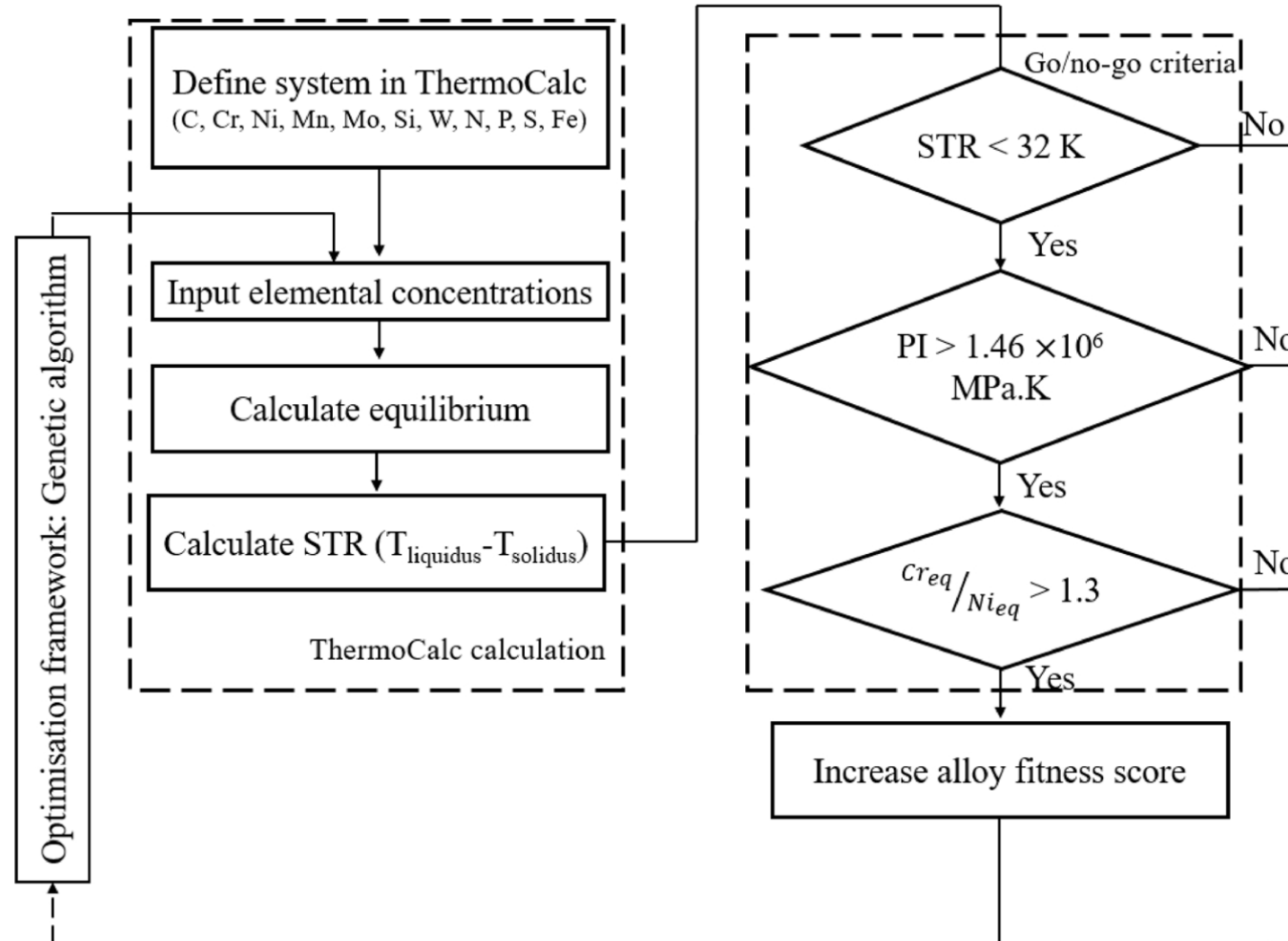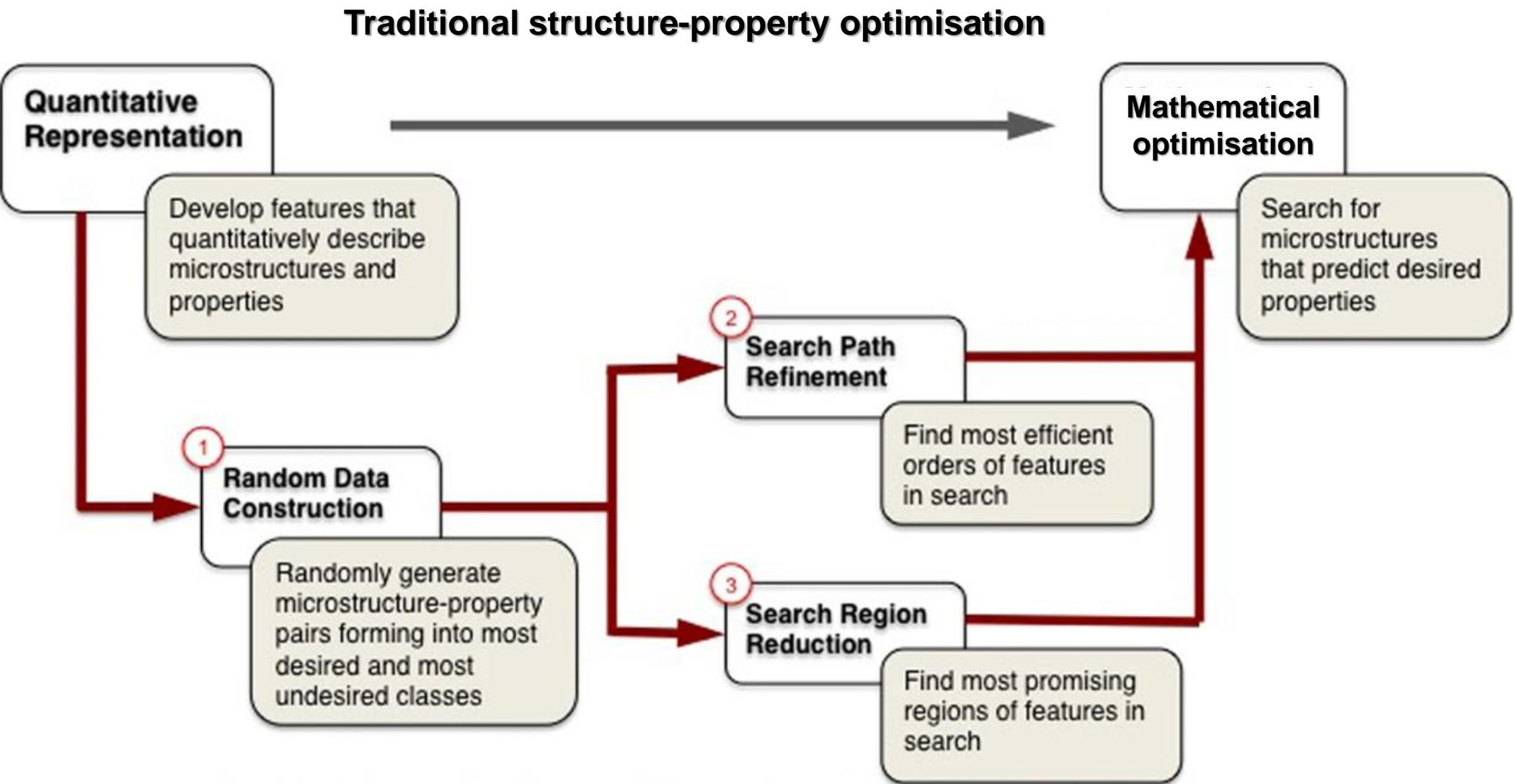
Optimisation methods

Fig. Algorithm for thermodynamic calculations and criteria evaluation using ThermoCalc

Optimisation methods

Traditional structure-property optimisation

Quantitative Representation

Develop features that quantitatively describe microstructures and properties

Mathematical optimisation

Search for microstructures that predict desired properties

① **Random Data Construction**

Randomly generate microstructure-property pairs forming into most desired and most undesired classes

② **Search Path Refinement**

Find most efficient orders of features in search

③ **Search Region Reduction**

Find most promising regions of features in search

Machine learning-based structure-property optimisation

Source: Liu et al. 2015 [DOI: 10.1038/srep11551]

Optimisation methods

Fig. Machine Learning based optimization

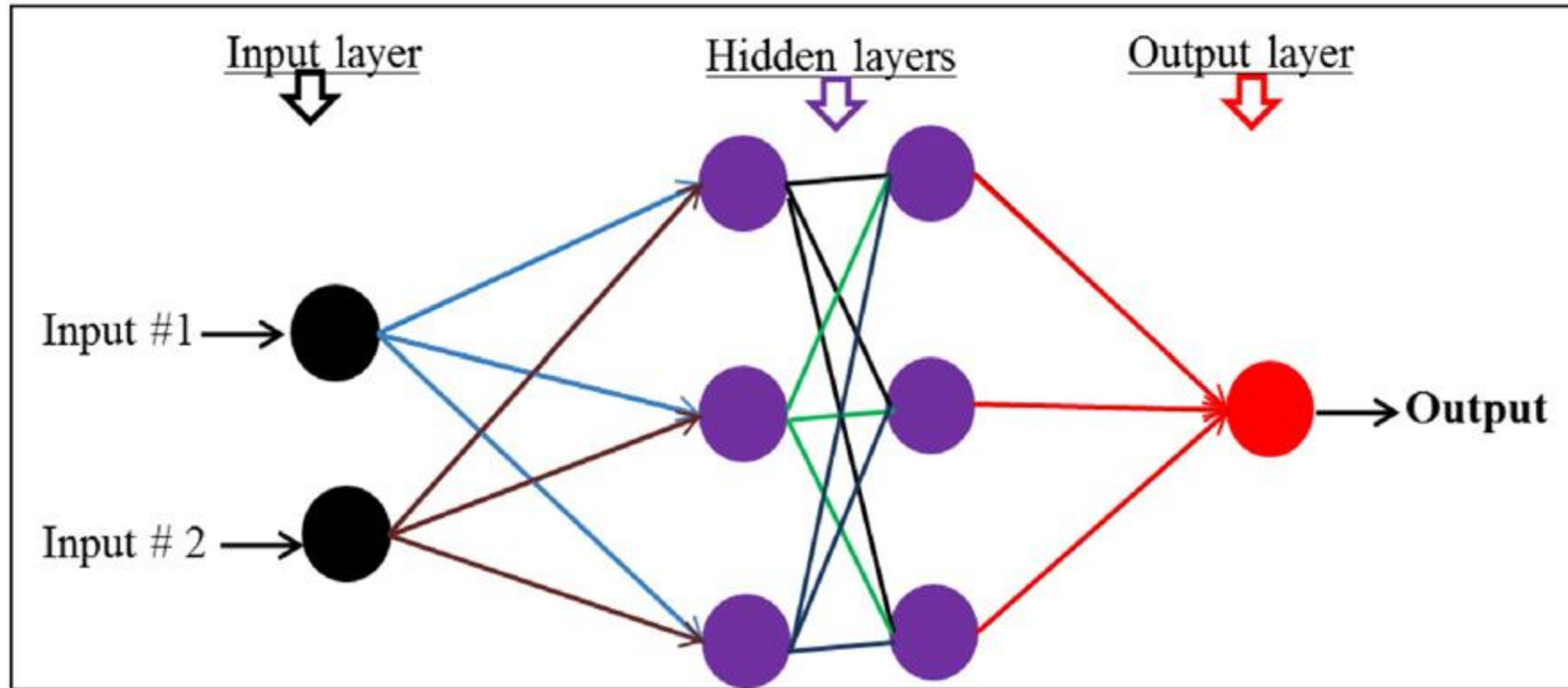Source: Meng et al. 2020 [https://doi.org/10.1007/s11837-020-04155-y]
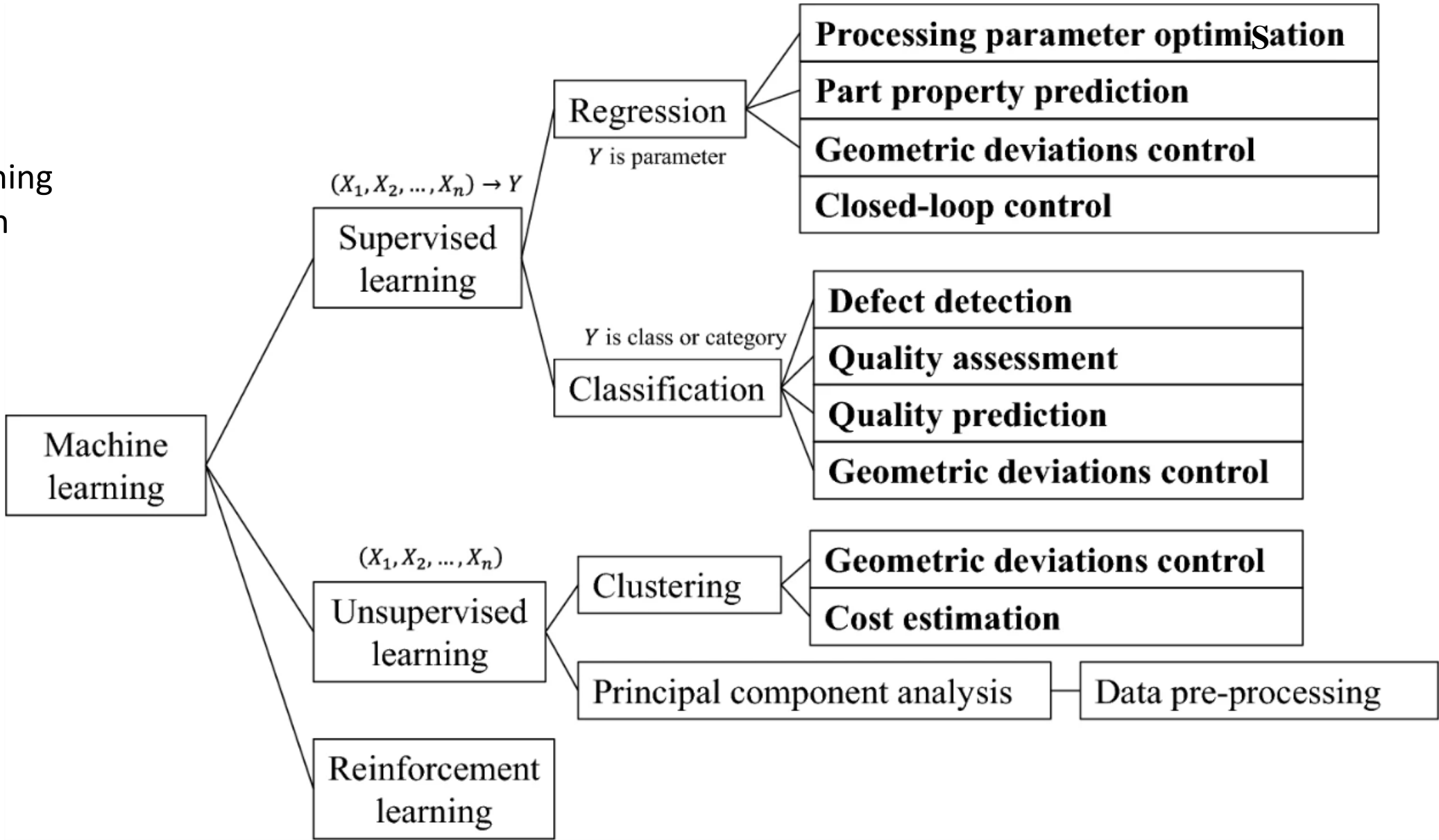
Optimisation methods

Fig. Schematic neural network model

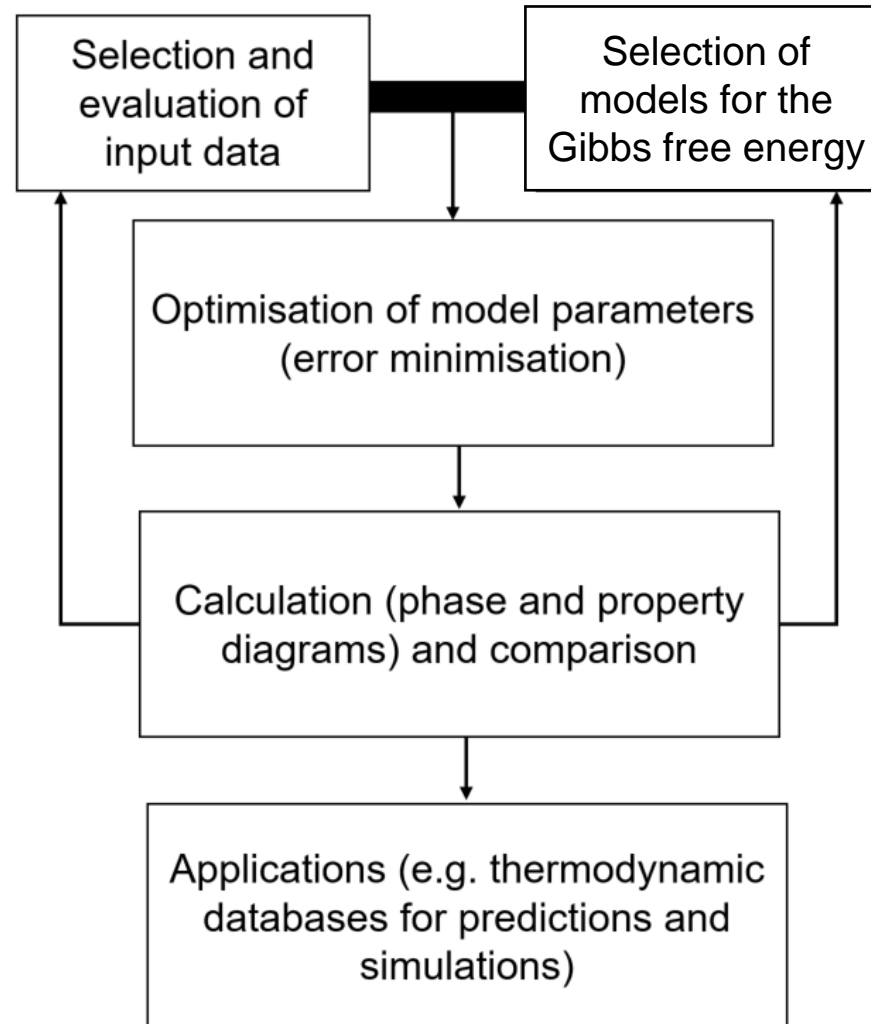# CALPHAD methodology

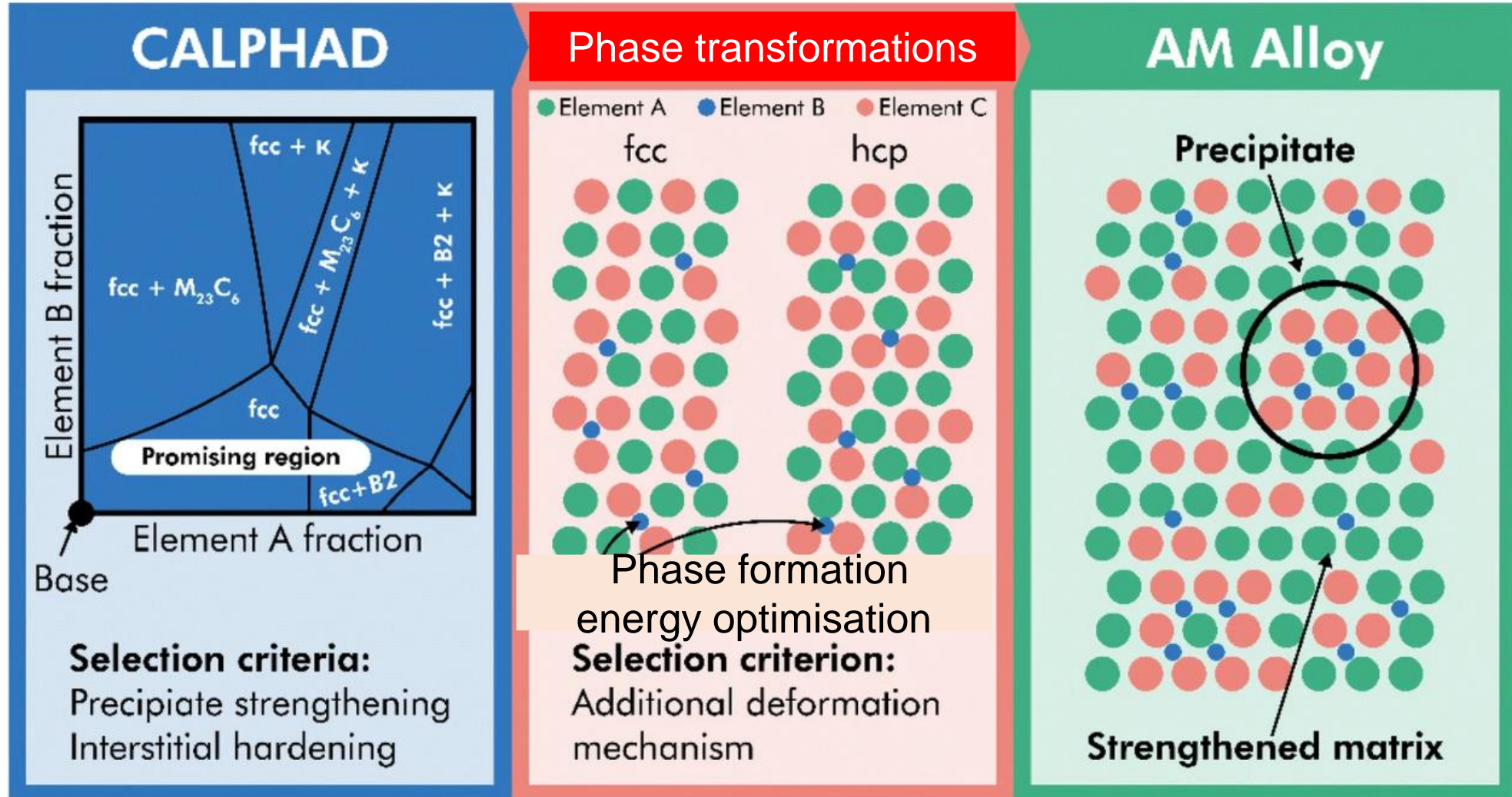**Fig.** Flowchart of Calculation of phase diagrams (CALPHAD) method

CALPHAD methodology

Fig. Schematic alloy selection approach using calculation of phase diagrams (CALPHAD) and phase transformations methods
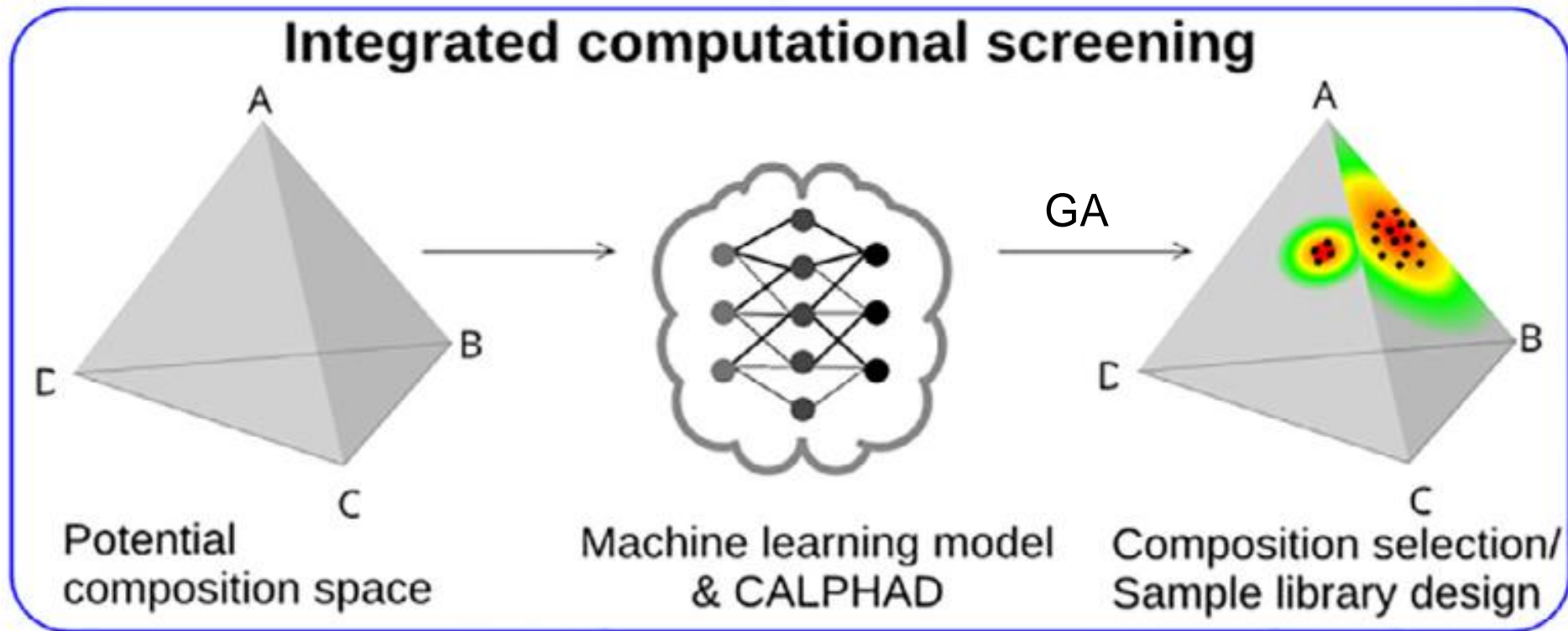
Source: Motaman et al. 2020 [https://doi.org/10.1007/s11837-020-04028-4]

Alloy design by combinatorial optimisation

Fig. Integrated computational screening using CALPHAD and machine learning models