# The HEA Project:

HEA - High Entropy Alloys
Development of a thermodynamic database to investigate new High-Entropy Alloys for High-Temperature applications and/or biomaterials

Experimental Part: Chemistry Department (DCCI) – Section of Inorganic Chemistry

Contact Persons:

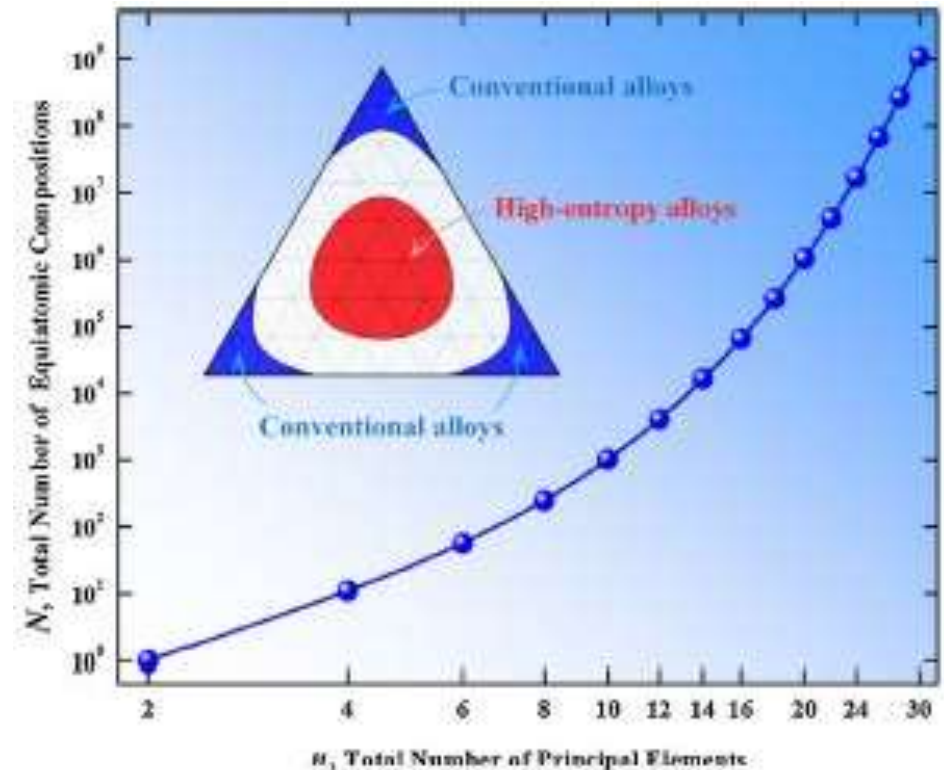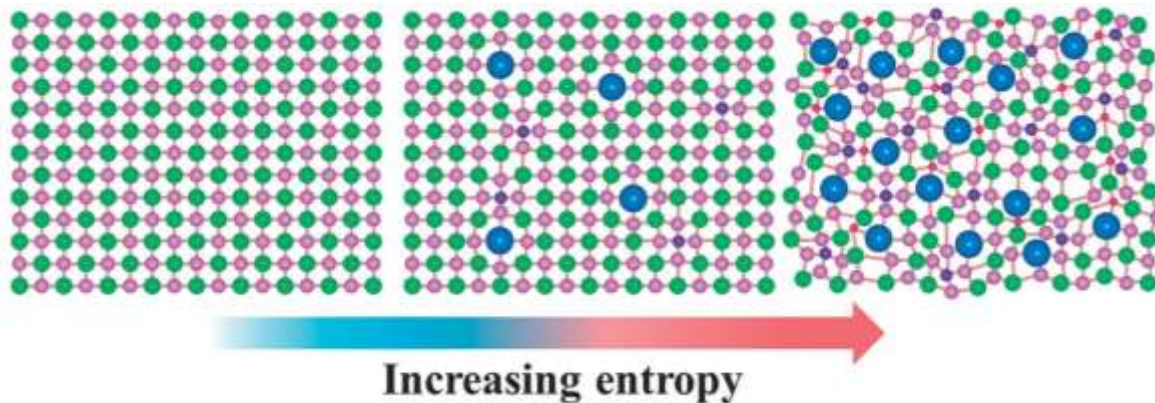Gabriele Cacciamani - Gabriele.Cacciamani@unige.it

Lorenzo Fenocchio - lorenzo.fenocchio@edu.unige.it
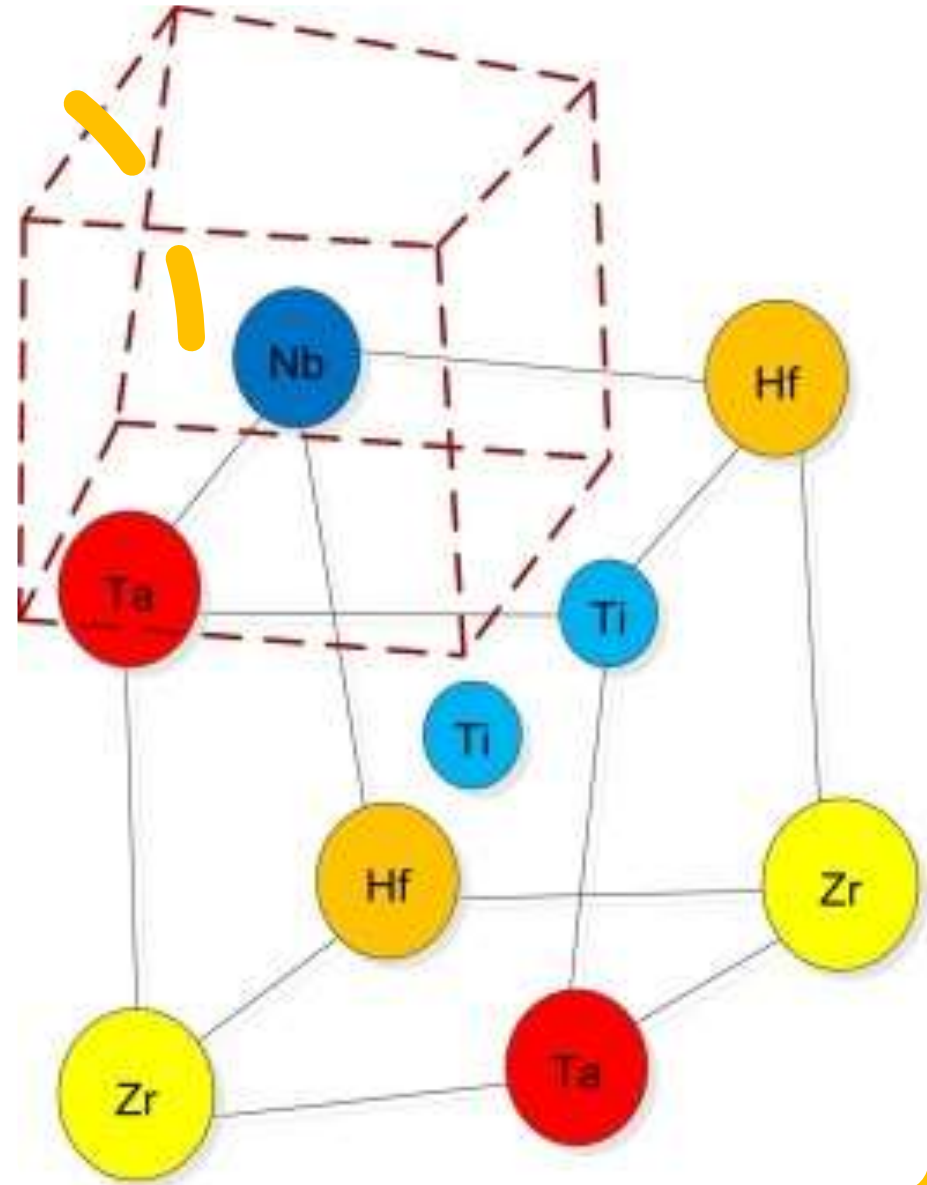
High Entropy Alloys (HEAs)

Innovative Alloys (2004, Yeh J. W. et al) characterized by:

- High number of components (≥5) in ~ equimolar quantities;

- High ideal configurational entropy (≥1.61R)

Increasing entropy

Ye Y.F. et al., "High entropy alloys: challenges and prospects", Materials Today 19 (2016), p. 349-363.
Jiang B. et al., "High entropy stabilized chalcogenides with high thermoelectric performances", Science 371 (2021), p. 830-834.

The HEAs Core Effects

High Entropy: favours formation of solid solutions over Intermetallics

Lattice Distortion: results from the differences between components and increases the entropy

Slow Diffusion: given by amorphous phases and precipitates forming during the synthesis

Cocktail Effect: the final alloy properties are better than the ones of the constituents

Building The Thermodynamic Database

Thermodynamic Simulations: Our Approach – The CALPHAD Method

Construction of the thermodynamic database

Extrapolation of multicomponent systems

Experimental validation of the performed predictions

Use of the database to simulate complex alloys for applications
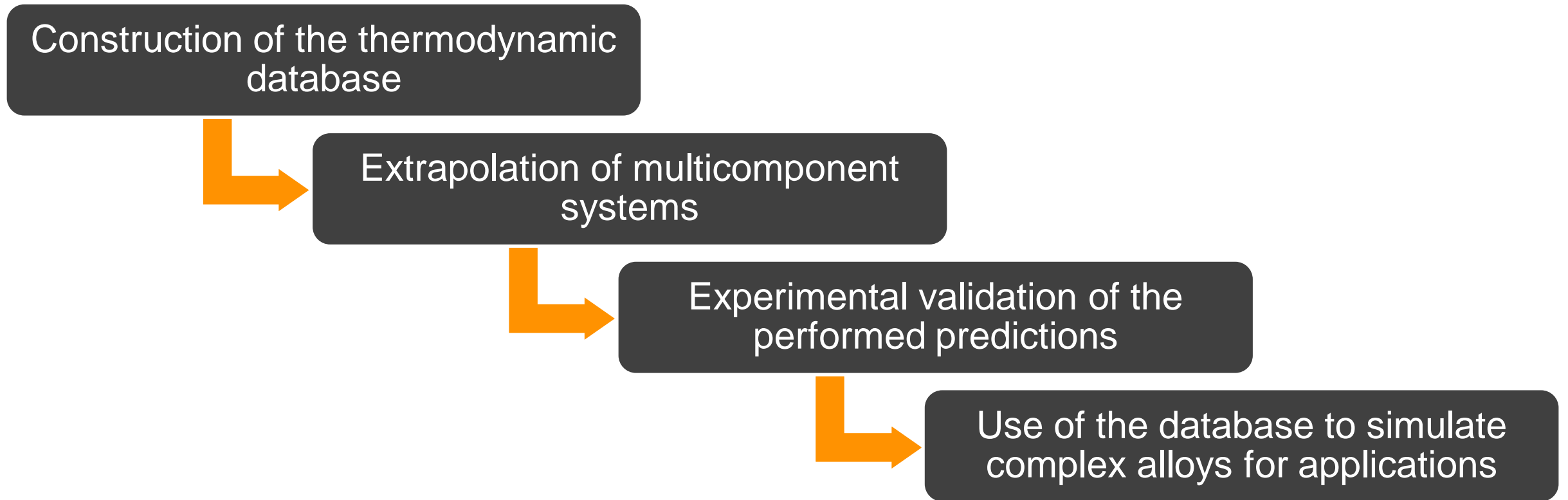
Example: The quinary Al-Cr-Co-Fe-Ni System

Experimental Part: The Al-Cr-Co-Fe-Ni System

- **Al** → Literature data validation
- **Co**, **Cr**, **Fe** → Experimental validation

1. Synthesis in Vacuum Arc Furnace from pure elements
2. Annealing for 90 days at 1050°C + Air Cooling
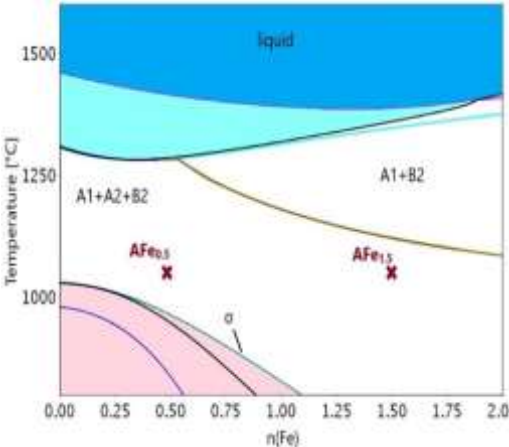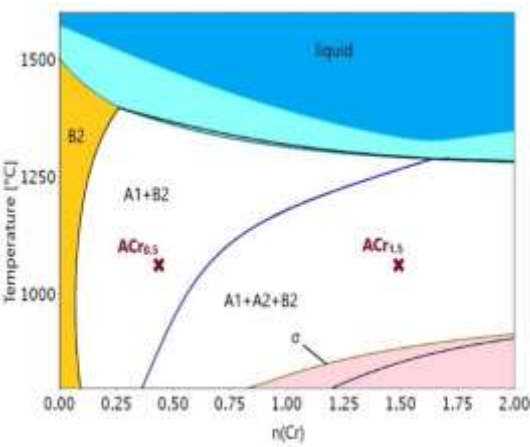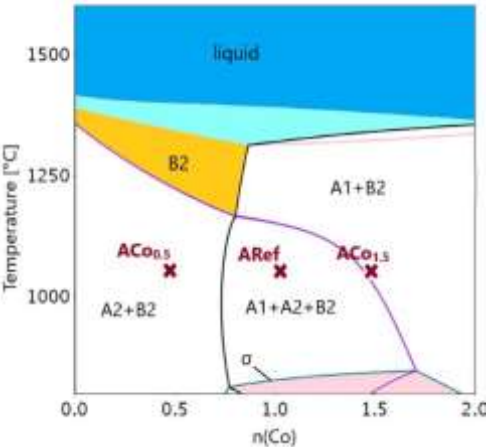3. XRD and SEM Analysis
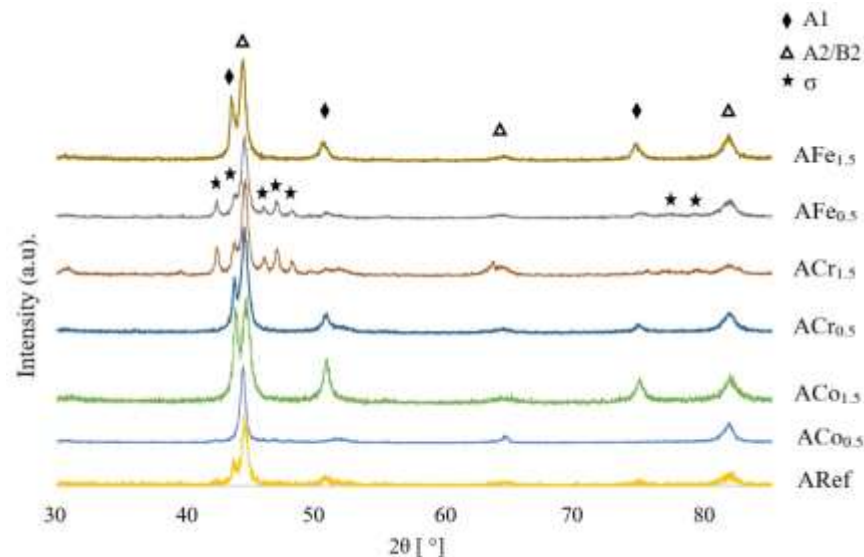
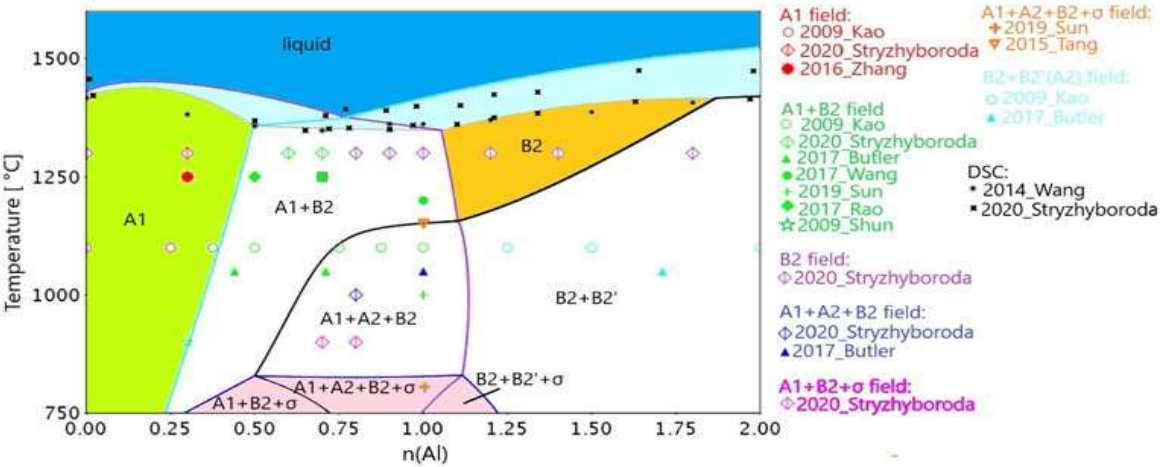| Sample	Nominal composition [mol]
ARef	Al-Co-Cr-Fe-Ni
ACo0.5	Al-$Co_{0.5}$-Cr-Fe-Ni
ACo1.5	Al-$Co_{1.5}$-Cr-Fe-Ni
ACr0.5	Al-Co-$Cr_{0.5}$-Fe-Ni
ACr1.5	Al-Co-$Cr_{1.5}$-Fe-Ni
AFe0.5	Al-Co-Cr-$Fe_{0.5}$-Ni
AFe1.5	Al-Co-Cr-$Fe_{1.5}$-Ni
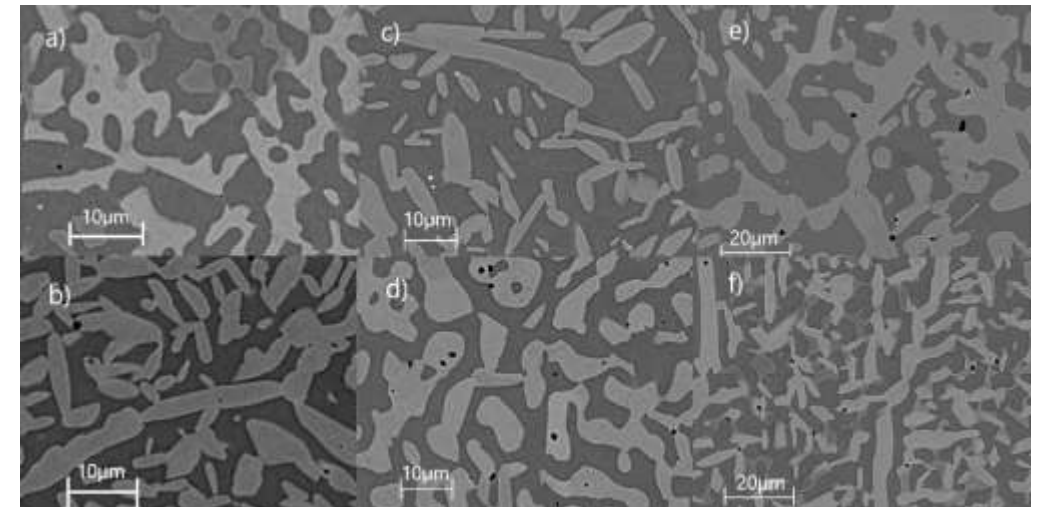
Phase Diagram Predictions – The Al-Cr-Co-Fe-Ni System

Experimental
Validation:

Multi-Component Phase
Diagram Prediction

Future Development

- Investigation (by calculations and experiments) of the refractory elements effect on HEAs – Mo, Ta, W

- Addition of Si to the database and experimental validation of the performed predictions