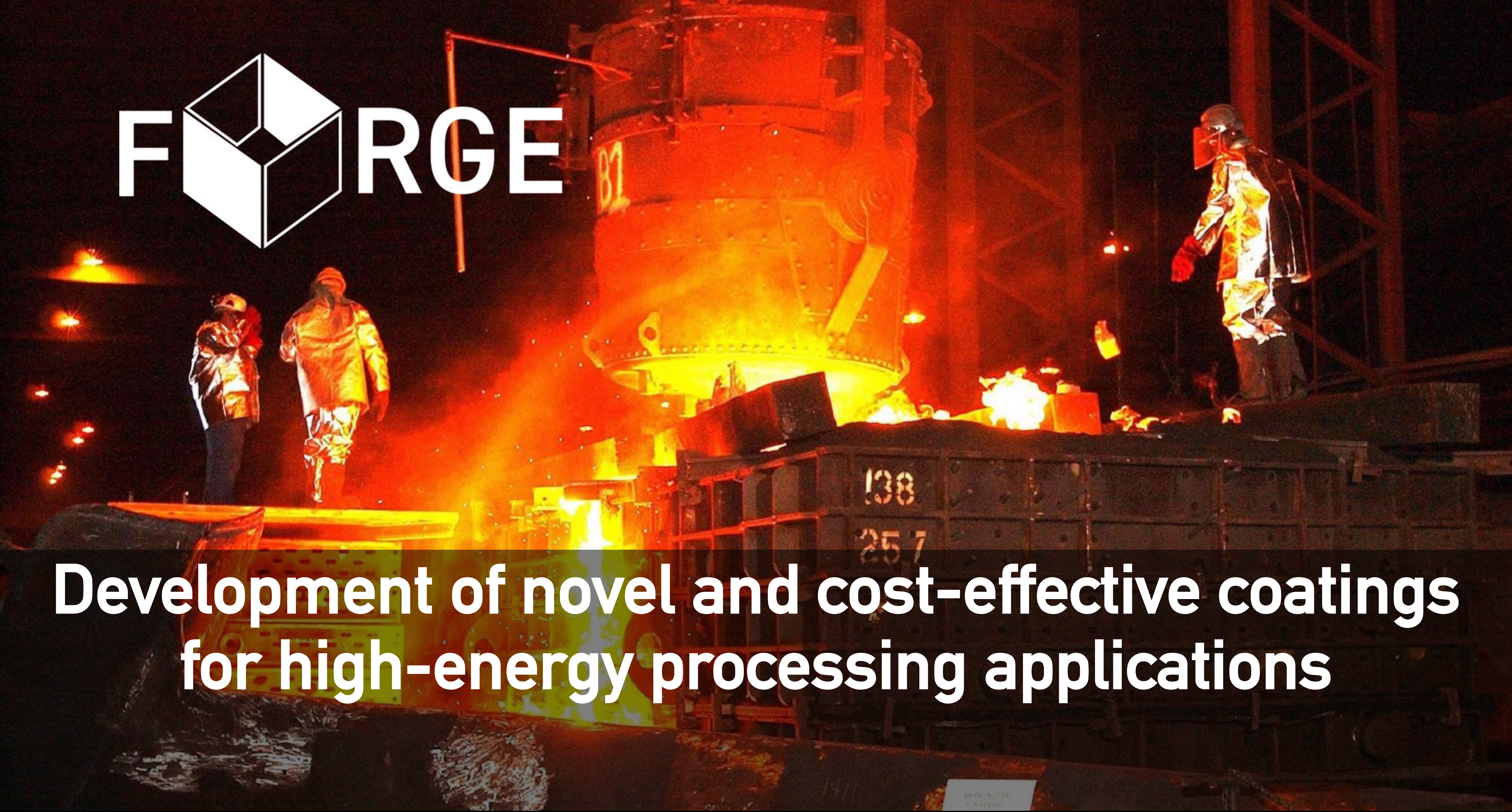

FORGE

Development of novel and cost-effective coatings for high-energy processing applications

This project has received funding from the European Union's Horizon 2020 research and innovation programme. Grant agreement 958457.

FORGE in numbers

Research Partners

- Empa Materials Science and Technology
- University of Leicester
- Fraunhofer ISC
- Max-Planck-Institut für Eisenforschung GmbH
- AeonX
- Technovative Solutions
- Cocas
- TWI
- Tailorlux integrity solutions
- MBN nanomaterialia

Industrial Partners

- AeonX
- Technovative Solutions
- Cocas
- TWI
- Tailorlux integrity solutions
- MBN nanomaterialia
- ASAŞ
- ÇİMSA
- AICE
- jtc
- Universitat Jaume I

13 Partners	5.9 M€
1st Nov 2020	42 months Apr 2024
648 Person Months	

www.forge-project.eu

This project has received funding from the European Union's Horizon 2020 research and innovation programme. Grant agreement 958457.

The Call for FORGE

Topic: **LC-SPIRE-08-2020 - Novel high performance materials and components (RIA)**

Specific challenges:

Overcome Materials inherent limitations that hinders Energy intensive industries to reach carbon neutrality by 2050.

Scope:

- **Design and Develop** highly innovative materials with improved properties
- Develop embedded sensor

Expected Impact:

FORGE Commitment:

30%

20%

Energy efficiency

Reduction of CO2 emissions

20%

40%

20%

24%

Increased lifetime

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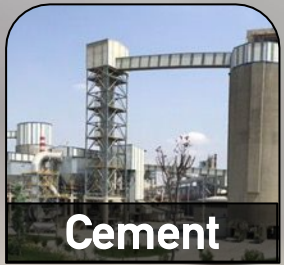

Application	Goal	Challenge
Cement	Waste heat recovery CO2 capture	high temperatures, acid contaminants and abrasive particles
Steel	H2 FUELED STEEL-MAKING	hydrogen embrittlement of the pipework, heat exchangers etc.
Aluminum	Increased lifetime of extrusion die	With high silicon content friction increases, as temperature and wear on the die
Ceramic	Increase lifetime and reduce thermal loss in Kiln	Thermal breakdown of Kiln Bricks at pyrolytic temperatures

Performance Targets Resistance to:

- PT1 CO_2 CORROSION
- PT3 WEAR
- PT2 H_2 EMBRITTLEMENT
- PT3 WEAR
- PT3 WEAR
- PT4 THERMAL BREAKDOWN
- PT4 THERMAL BREAKDOWN
- PT1 CO_2 CORROSION

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Identified issues for EII

FORGE address the materials surface degradation problems found in energy-intensive industries, both now and in future, and focus on <u>four key problems (or Performance Targets)</u>:

PT1 CO_2

- **Corrosion** of metallic components from acidic, basic and reactive species in CCUS

PT2 H_2

- **Hydrogen embrittlement** of high-strength steels from hydrolytic and process hydrogen

PT3

- **Mechanical Damage**, such as erosion, impact damage of process plant from particulates, wear from friction

PT4

- **Thermal breakdown**, i.e. alkaline attack at pyrolytic temperatures, thermal degradation induced by friction etc

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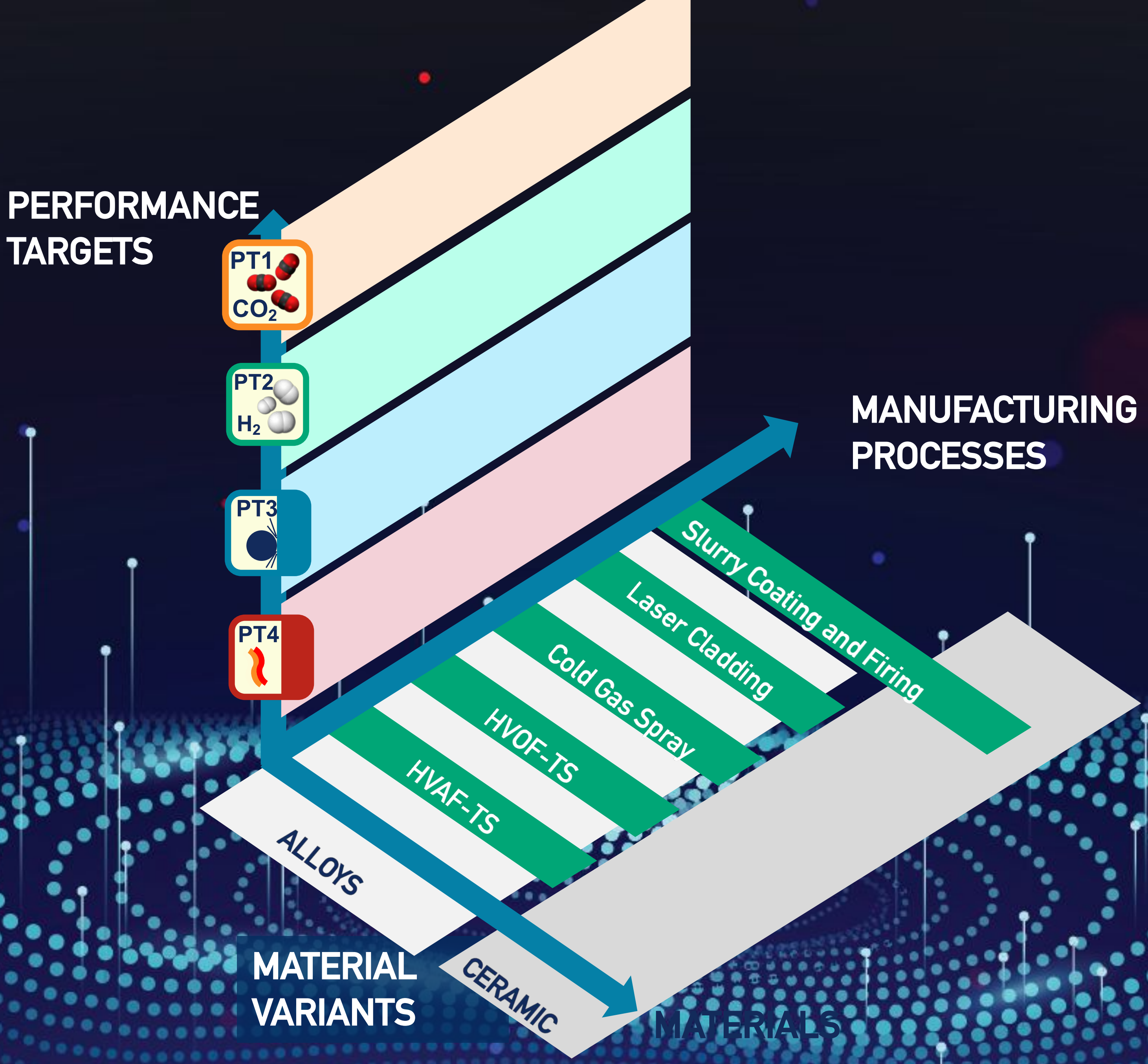

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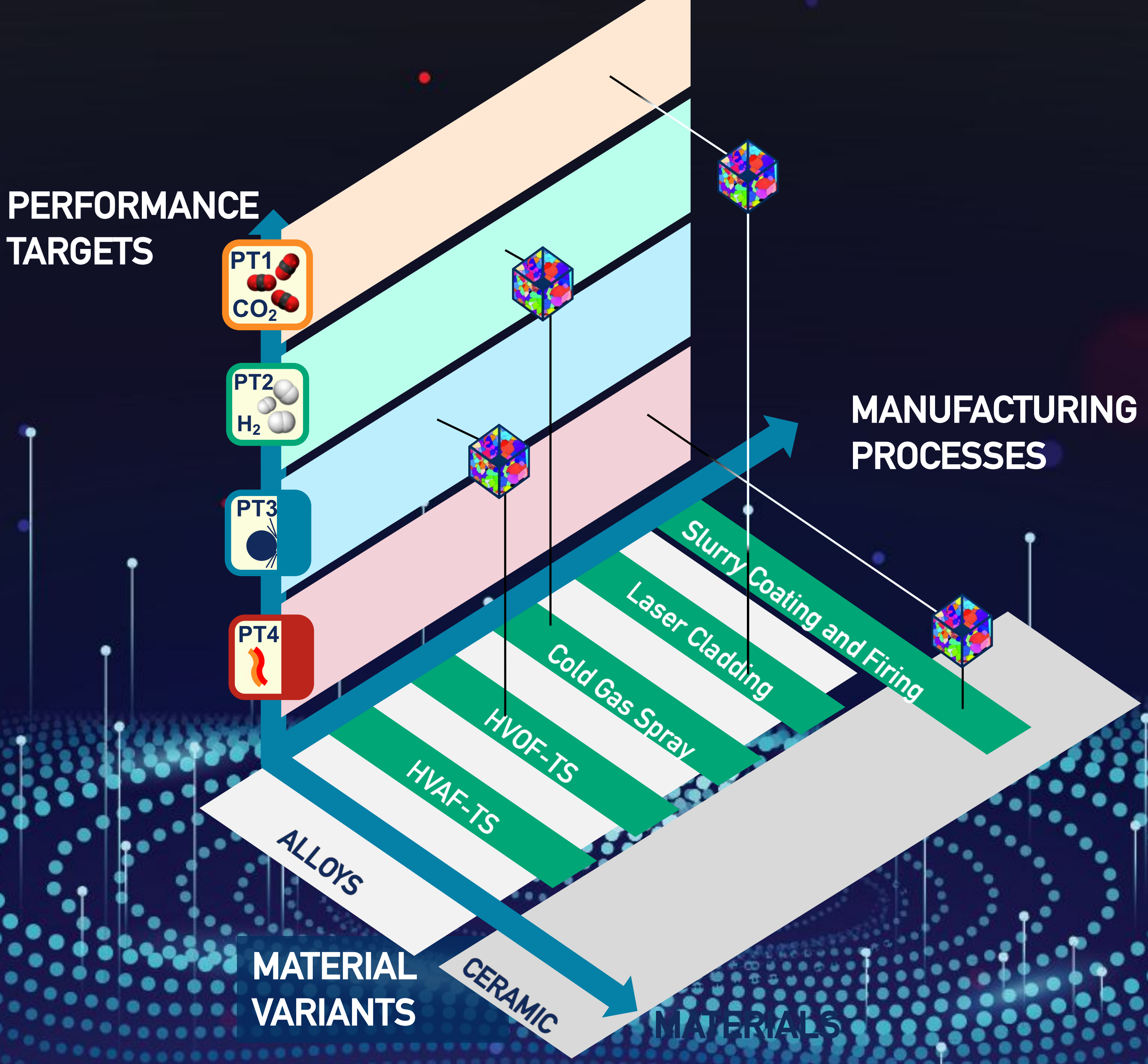

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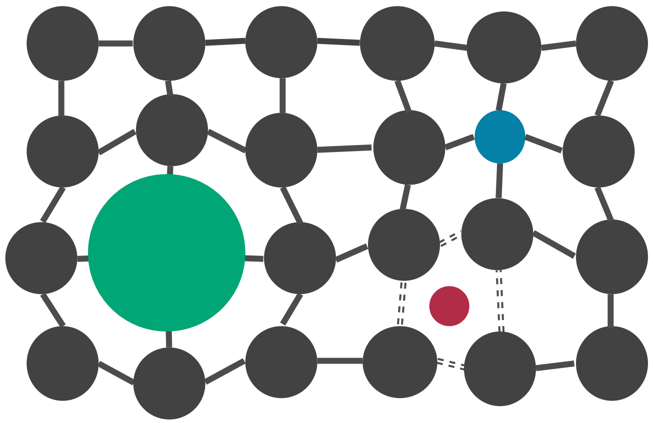
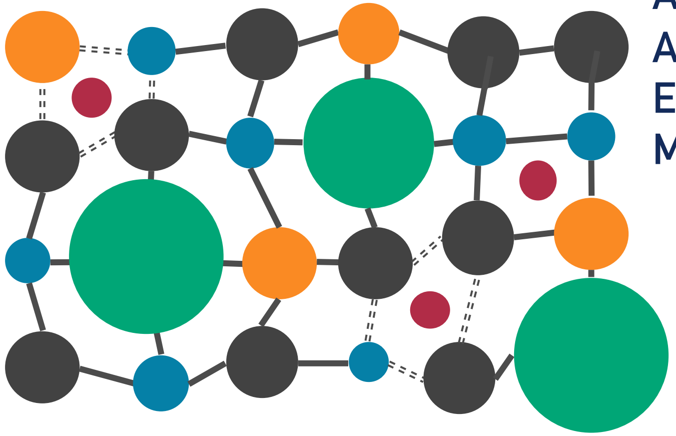
The New Materials from FORGE

Conventional Metal Alloys



Compositionally Complex Alloy



Alloys that have no dominant element
Alloys with more than 4 elements
Element concentration 5-40at%
More that one phase can be present

- **high configurational entropy and large lattice distortions**
  contribute in a unique way to the mechanical properties
- **good corrosion resistance**
  corrosion and pitting potentials in the range of austenitic and ferritic stainless steels
- **the ability to depart from alloy dominated by a single element offers the possibility to tailor new combination of material physical properties**

LINK

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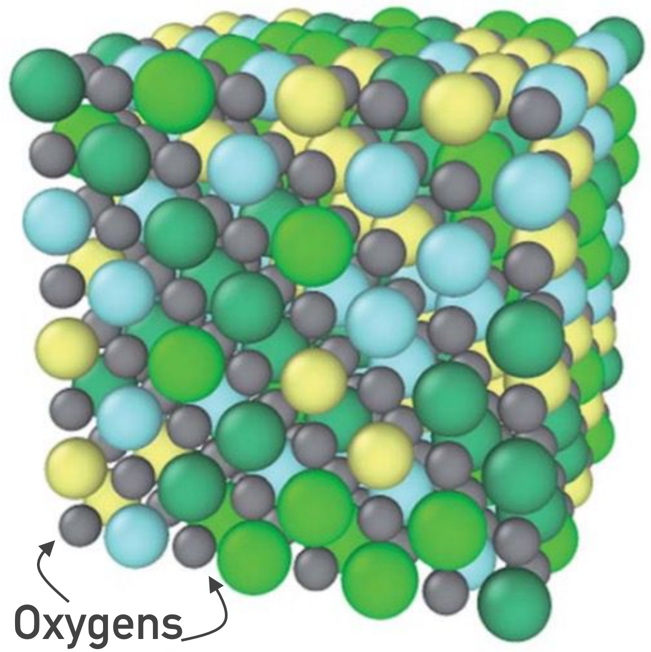
Compositionally Complex Ceramics



- Extend the range of the HEC-compounds to include medium entropy and non-equimolar compositions
- Lower thermal conductivities than their highly entropic counterpart
- Outperform HEC for their mechanical properties

LINK

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FORGE

Design Starting Point

H																	He
Li	Be											B	C	O	N	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Ab	Te	I	Xr
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pr	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Bd	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

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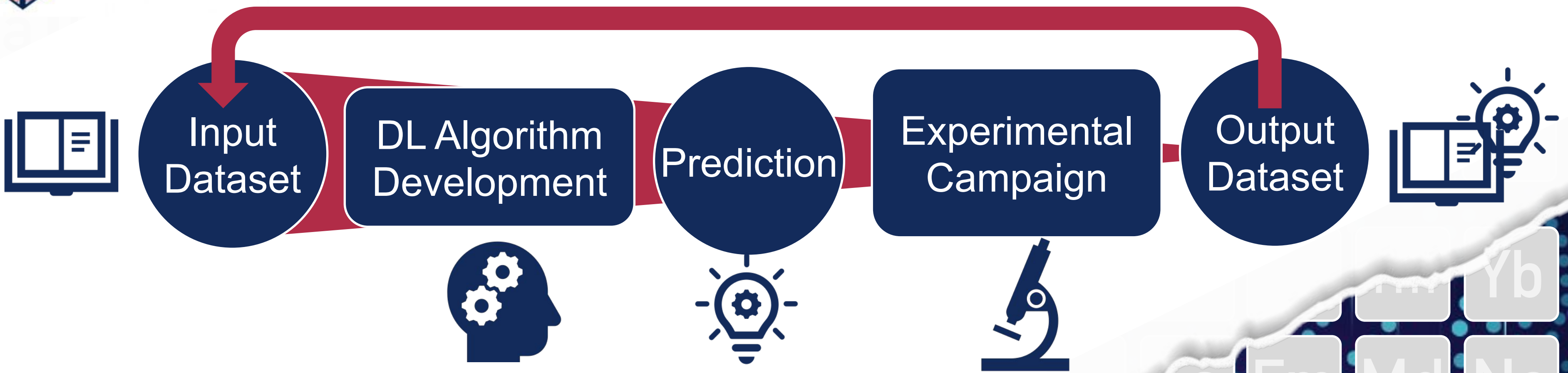
a systematic material development approach
=> impossible task, countless compositions

development is supported by Deep Learning algorithms able to correlate the properties and composition of CCA/CCC



…search and innovation programme. Grant agreement 958457.

FORGE Dataset Generation

Data	Example
Composition at.	$Al_{0.25}$ Co_1 Fe_1 Ni_1
Composition %	$Al_{7.6}$ $Co_{30.8}$ $Fe_{30.8}$ $Ni_{30.8}$
Phases (Measured)	FCC
Synth. Method	Casting
Hardness (Measured)	138 HV

Data from Open Repositories, Open access reviews and articles:
High Entropy Alloys, Compositionally Complex Alloys and High Entropy Ceramics systems

DATASET INTEGRATION	
Composition %	$Al_{7.6}$ $Co_{30.8}$ $Fe_{30.8}$ $Ni_{30.8}$
Phases (calculated)	FCC (fraction)
Liquidus-Solidus Temp.	1425-1412°C
Gibbs Energy (calculated)	-122270
Enthalpy (calculated)	38641
Entropy(calculated)	95,74
Helmotz Energy (calculated)	-122270
Yield strength (calculated)	94,13

Integration of the datasets with calculated parameters based on integration of CALculation of PHAse Diagrams (CALPHAD) method into Integrated Computational Materials Engineering (ICME) Approach

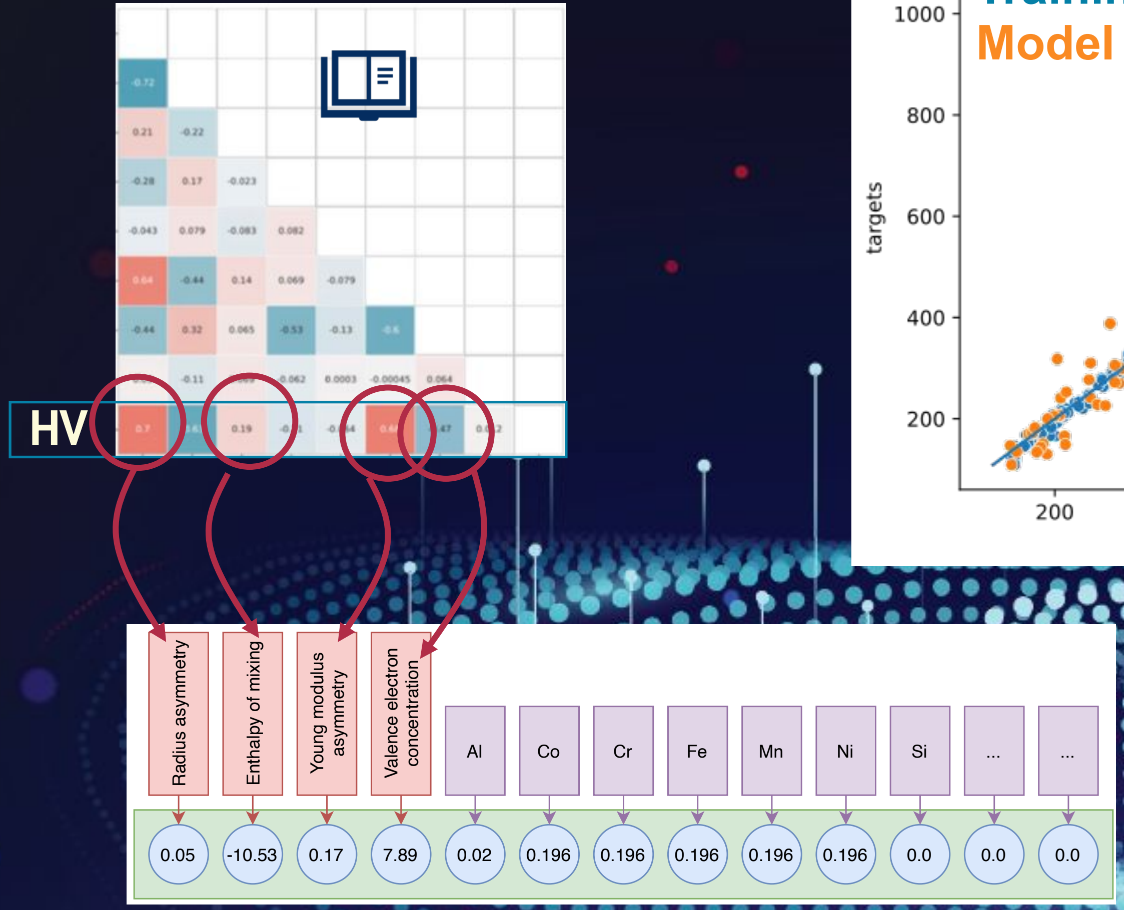
Radius Asymmetry	Entropy/Enthalpy ratio
Enthalpy of Mixing	Young modulus asymmetry
Entropy of Mixing	Valence electron Concentration
Mean Mealting Temperature	Electronegativity

Integration with parameters calculated directly from the composition and the element properties

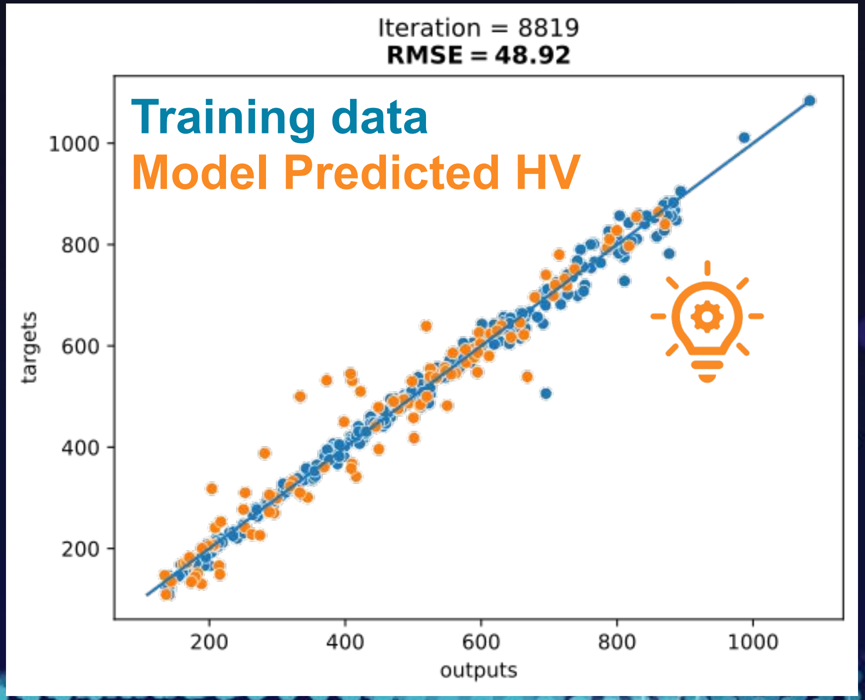
LINK

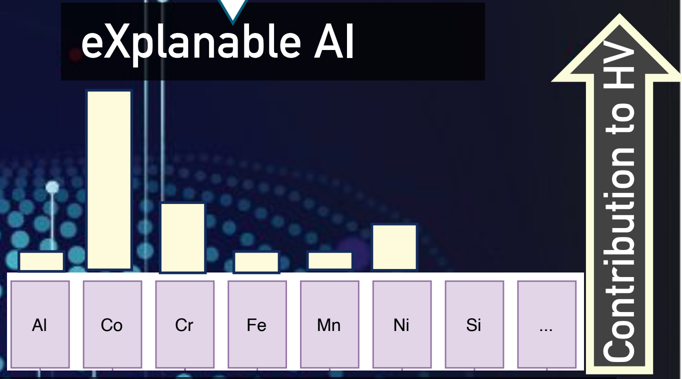
FORGE Strategy for Deep Learning

Correlation Matrix



Input Vector





To identify the underlying relation between CCA/CCC input features and DL estimated properties

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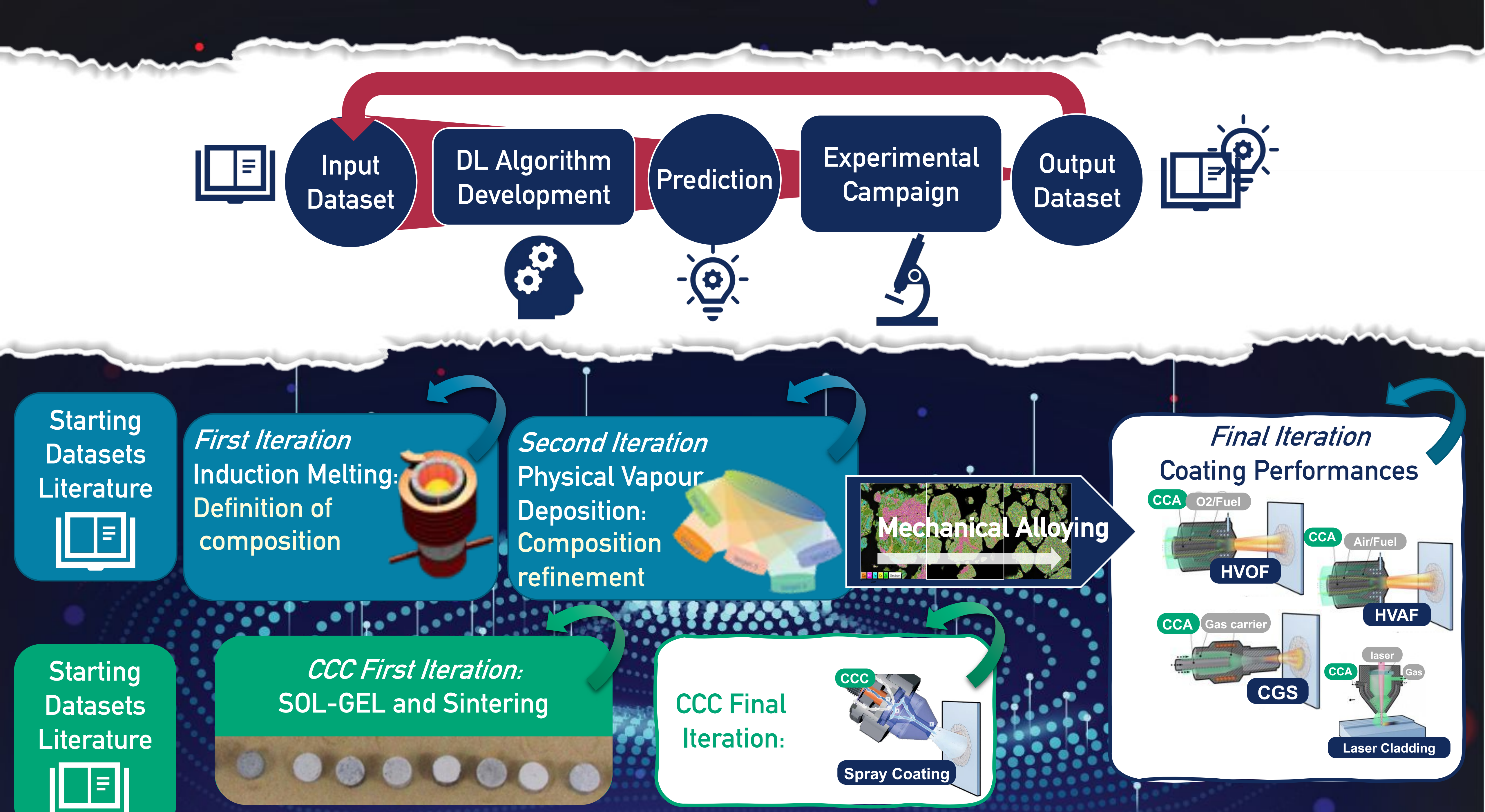

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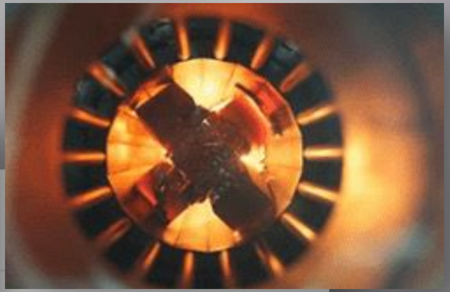
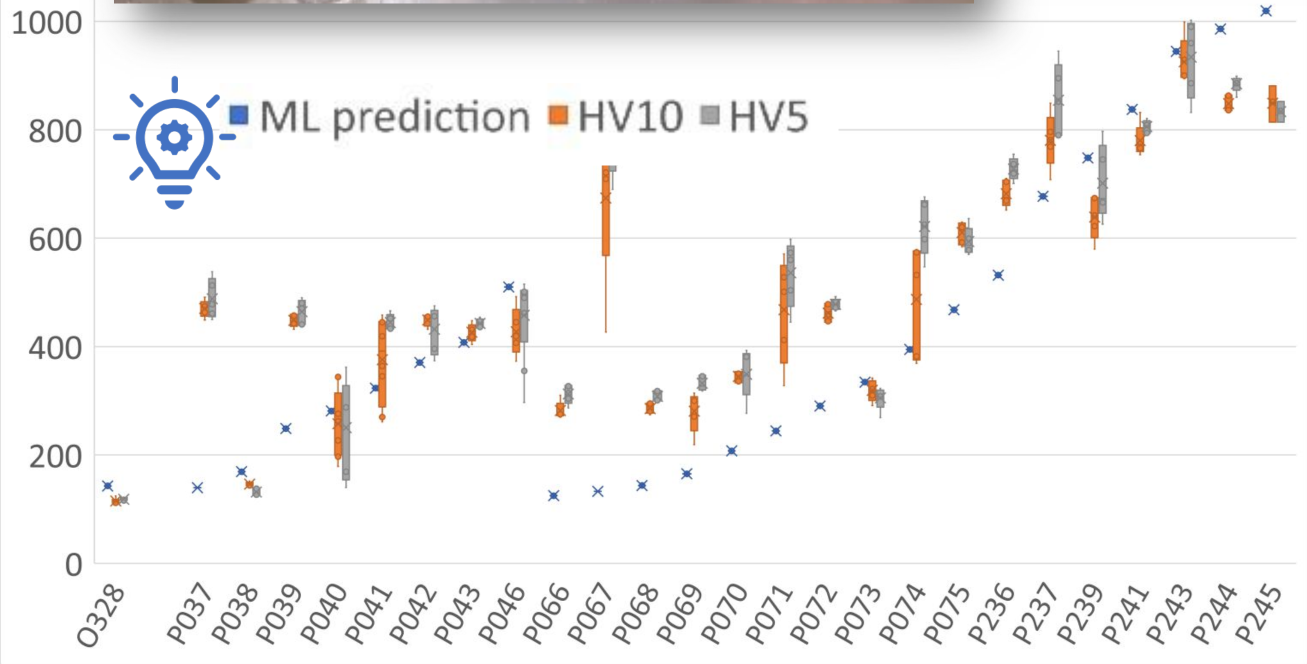
Experimental Campaigns

Bulk Specimens from Induction Melting and Casting



- 30 alloys from first ML-predictions have been synthetized
- Melting CCAs is a challenge, broad melting temperatures (Al660° W3600°), reactive with crucibles (Ti)
- First feedback of the DL-algorithm predictions
- Specimens from these 30 new alloys are being tested for HV, Corrosion, and H2 embrittlement



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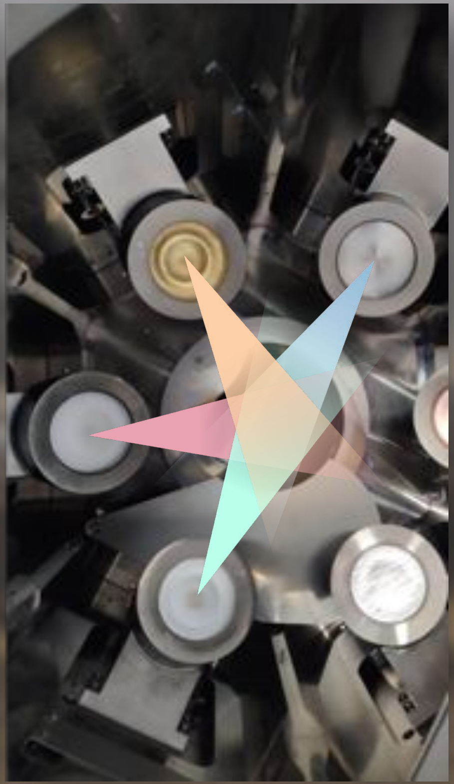
Coatings by Physical Vapour Deposition

To synthesize hundreds of alloys in a single process by combinatorial deposition in the same wafer

Element gradients will be defined considering the output of eXplainable AI, for the most relevant Element

Reference Composition (Cantor) have been produced and distributed for preliminary tests



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Experimental Campaigns

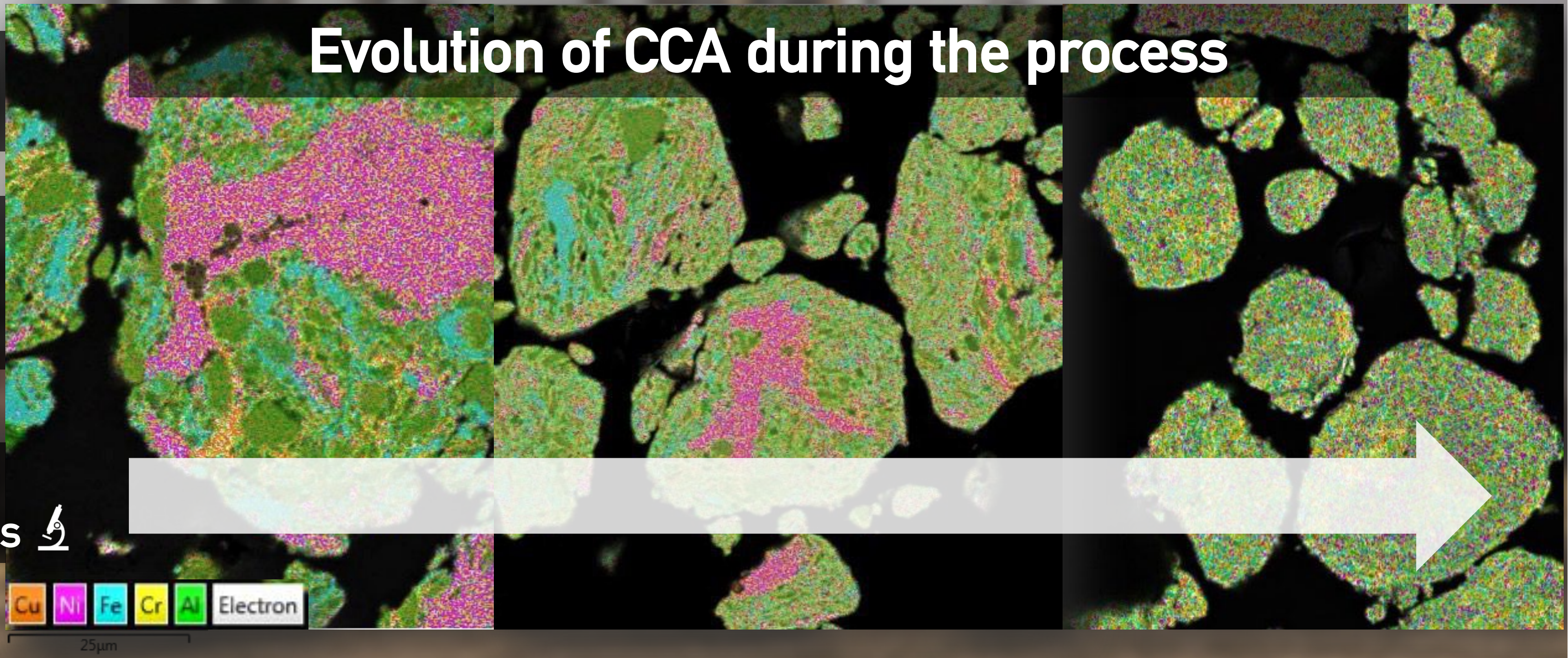
Powders from Mechanical Alloying

Mechanical Alloying output is a powder and gives more flexibility in the CCA composition

Diverse composition has been tested to define the strategies for CCA containing ductile and refractory elements

Reference Composition (Cantor) have been produced and distributed for preliminary tests

Evolution of CCA during the process



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LINK

Compositionally Complex Ceramics

Data in literature are not as available as for the Alloys, i.e. no reviews collecting CCC and their CTA

DL-algorithms purely based on calculated properties (i.e. AFLOW) are self-referential

More than 80 composition has been synthesized in the attempt to create an internal database

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KPI number	KPI Name	Tested by	Test name (standard)	Quantity measured directly from test	KPI	KPI target value	KPI Units
WP2							
2,1	Hardness	ARC	Vickers hardness (ASTM E92)	Hardness (HV10)	Deviation from ML predicted hardness	<10	%
2,2	H_2 charging	ARC	charging via a solution containing (hydrogen or deuterium) + Thermal Desorption Spectra (TDS) (diffusible hydrogen)	H_2 content after charging (ppm)	H_2 content after charging (ppm)	<SOA value	ppm
2,3	HNO_3 resistance (cast specimens)	TWI	Linear Polarisation Resistance (ASTM G59/G102)	Corrosion rate (mm/y)	Corrosion rate	<0.1	mm/y
2,4	Nanohardness	EMPA	Nanohardness (ISO 14577)	Hardness (HV)	Deviation from ML predicted hardness	<10	%
2,5	H_2 charging	MPI	Hydrogen charging followed by nanoindentation (customised test)	Hardness (HV)	Hardness variation	<10	%
2,6	HNO_3 resistance (PVD patterns)	TWI	Droplet corrosion (customised test)	Corrosion rate (mm/y)	Corrosion rate (thickness loss)	<1	mm/y
2,7	Cost	MBN	n/a	Cost (€/kg)	Cost	<30	Cost (€/kg)
WP3							
3,1	Porosity (sol route)	Fraunhofer	Archimedes mehod (DIN EN 623-2)	Porosity (vol%)	Porosity	<5	vol. %
3,2	Corrosion rate	Fraunhofer	Microstructural analysis after corrosion exposure (customised)	Corrosion rate (mm/y) from (mm/run)	Corrosion rate (CCC-coated refractory	<0.5	[-]
3,3	CTE (sol route)	Fraunhofer	Dilatometry (DIN EN 821)	CTE (10^{-6}/K)	Deviation from brick CTE	<200 CTE (coating)-CTE (brick) < +-	%
3,4	Porosity (powder route)	Fraunhofer	Archimedes method (DIN EN 623-2)	Porosity (vol%)	Porosity	<5	vol. %

Key Performance Targets

Forge Definited the Acceptable Threshold at each development stage down to industrial validation

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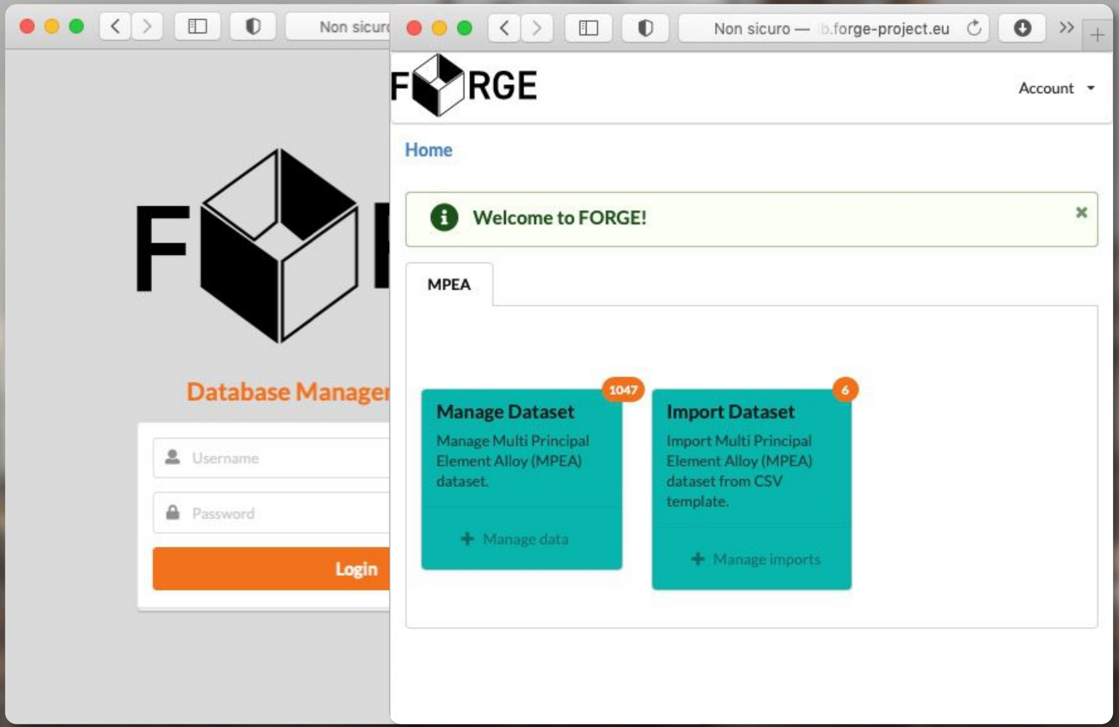
Centralized Database

FORGE



Formula (Mol. Ratio)	Property: Microstructure	Property: Processing method	Property: Grain size (µm)	Property: Exp. Density (g/cm³)	Property: Calculated Density	Property: HV	Property: Type of test	Property: Test temperature (°C)	Property: YS (MPa)	Property: UTS (MPa)	Property: Elongation (%)	Property: Elongation plastic (%)	Property: Exp. Young modulus (GPa)	Property: Calculated Young modulus (GPa)	Property: O content (wppm)	Property: N content (wppm)	Property: C content (wppm)	Reference: doi	Reference: year	Reference: title

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Questions ?

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