FUNMIN

FUNdamental Studies of **MIN**eral Carbonation with Application to CO_2 Utilisation

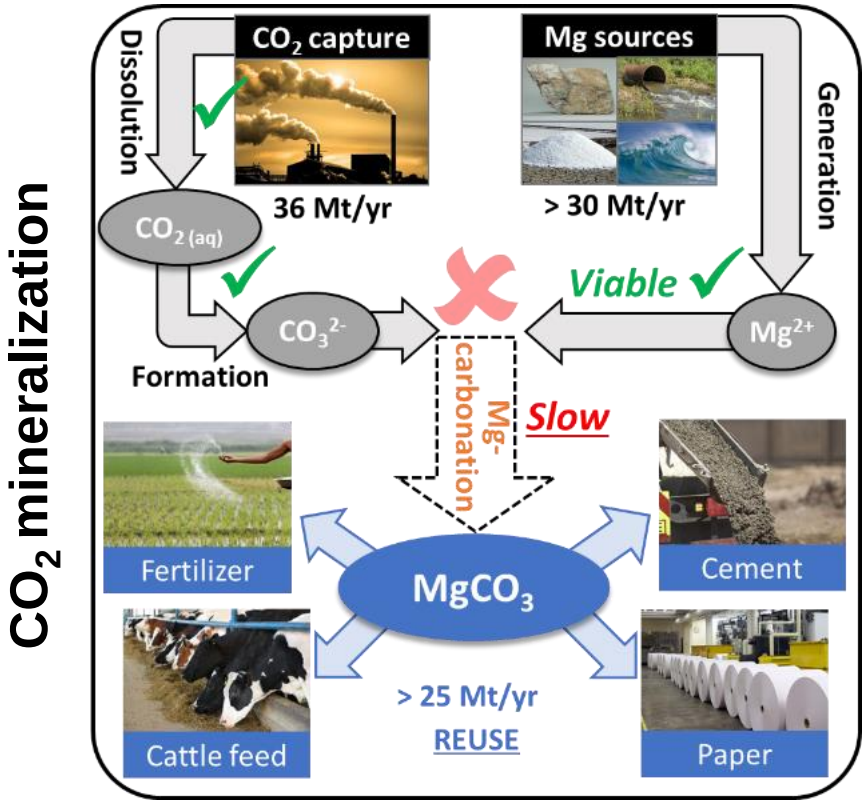
By Devis Di Tommaso, Queen Mary

Presented at ACT workshop

07.11.2019

CO_2 into added-value products

"CCUS can create new industries and markets through the use of carbon dioxide, such as chemicals, plastics, and building materials" *



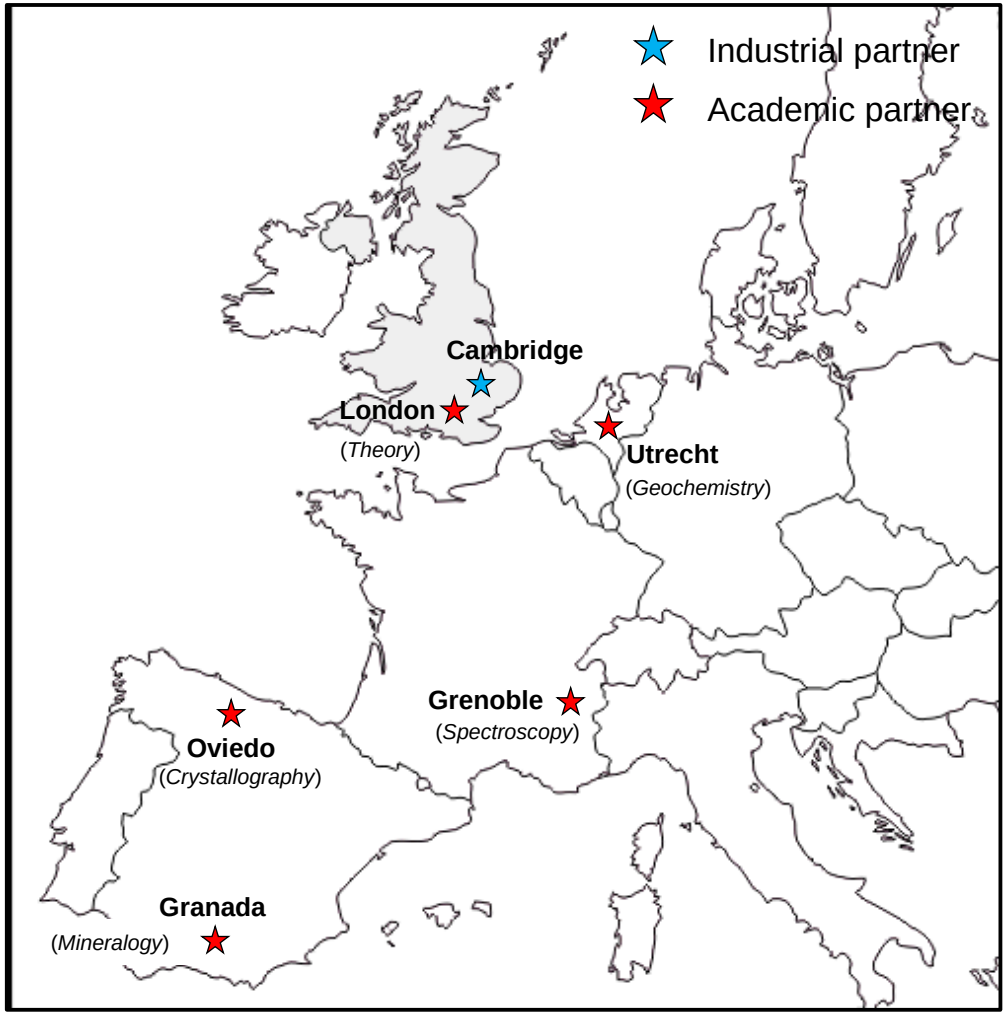
Cambridge Carbon Capture Ltd technology (**CO2LC**) to store CO_2 in mineral form ($MgCO_3$)

* The UK carbon capture, usage and storage (CCUS) deployment pathway, BEIS, 2018

The FUNMIN consortium

World expertise in mineralization guiding Industrial technologists
to permanently mineralise CO_2

$$\mathbf{CO_{2\,(gas)} \rightarrow MgCO_{3\,(solid)}}$$



Queen Mary University of London

Cambridge Carbon Capture

Utrecht University

UNIVERSIDAD DE GRANADA

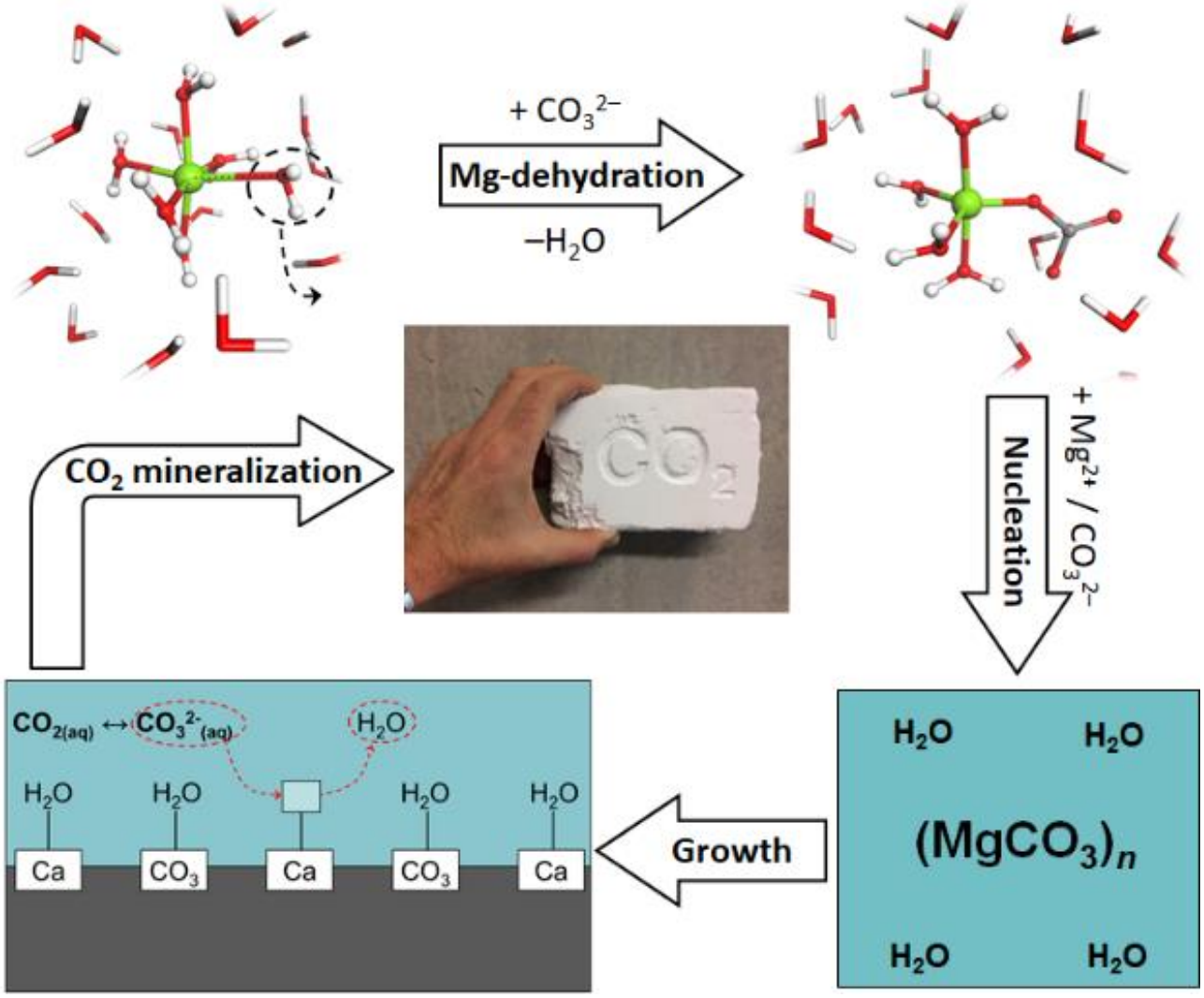
Universidad de Oviedo
Universidá d'Uviéu
University of Oviedo

UGA Univ. Grenoble Alpes

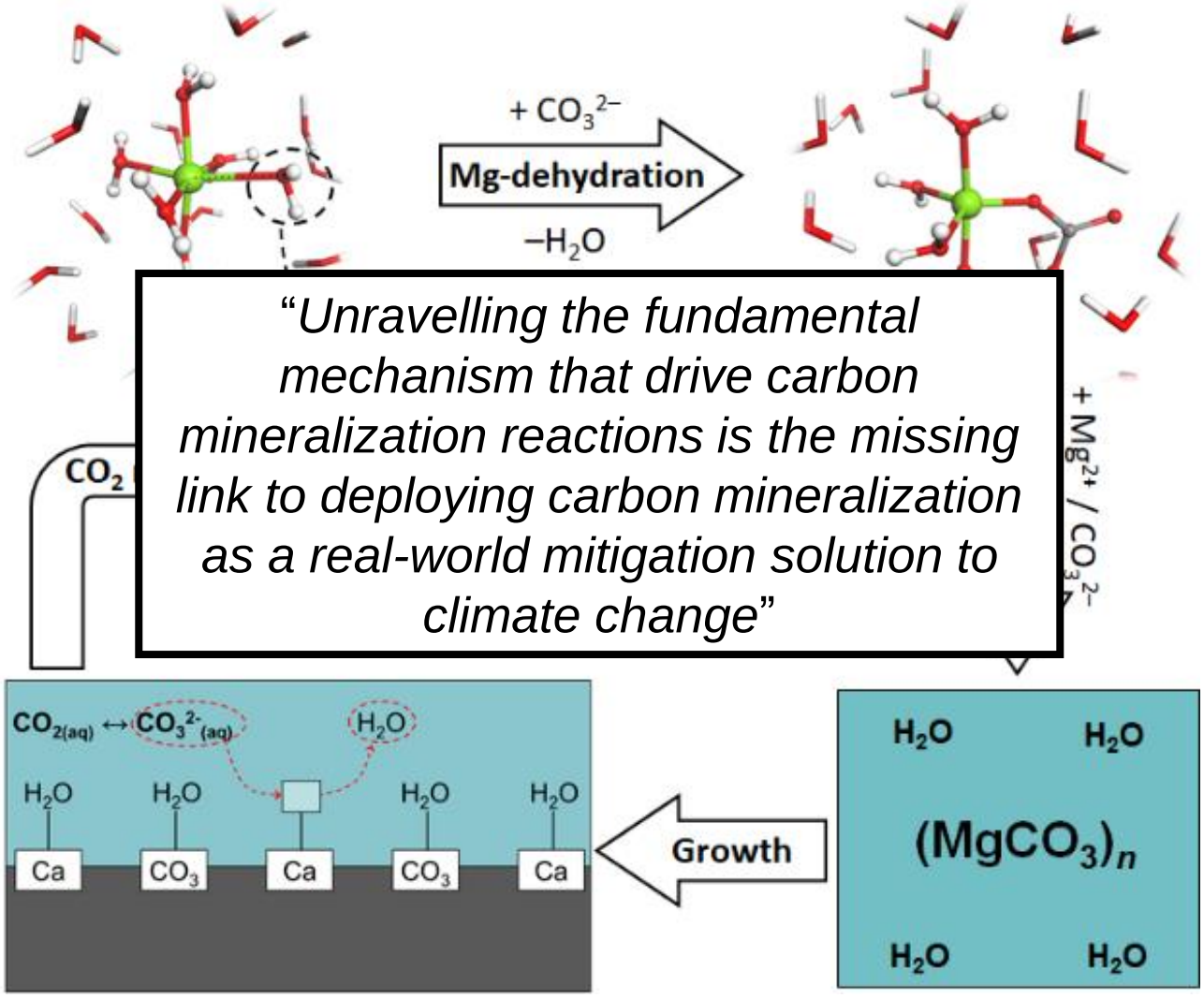
FUNMIN facts

- Full Economic Cost: **€ 890k** (€ 700k from ACT + € 190k in-kind)
- Duration: **30 months** (10/2019 – 03/2022)
- Academic partners: **QMUL** (coordinator), **UGR**, **UO**, **UGA**, **UU**
- Industrial partner: **Cambridge Carbon Capture Ltd**
- Associate partners: National Physical Laboratories (UK), McMaster University (Canada), University of Hong Kong (China), Seoul National University (Korea)
- **ISIS Neutron and Muon Source facility** at Rutherford Appleton Laboratory (UK)

Mineral carbonation



Mineral carbonation

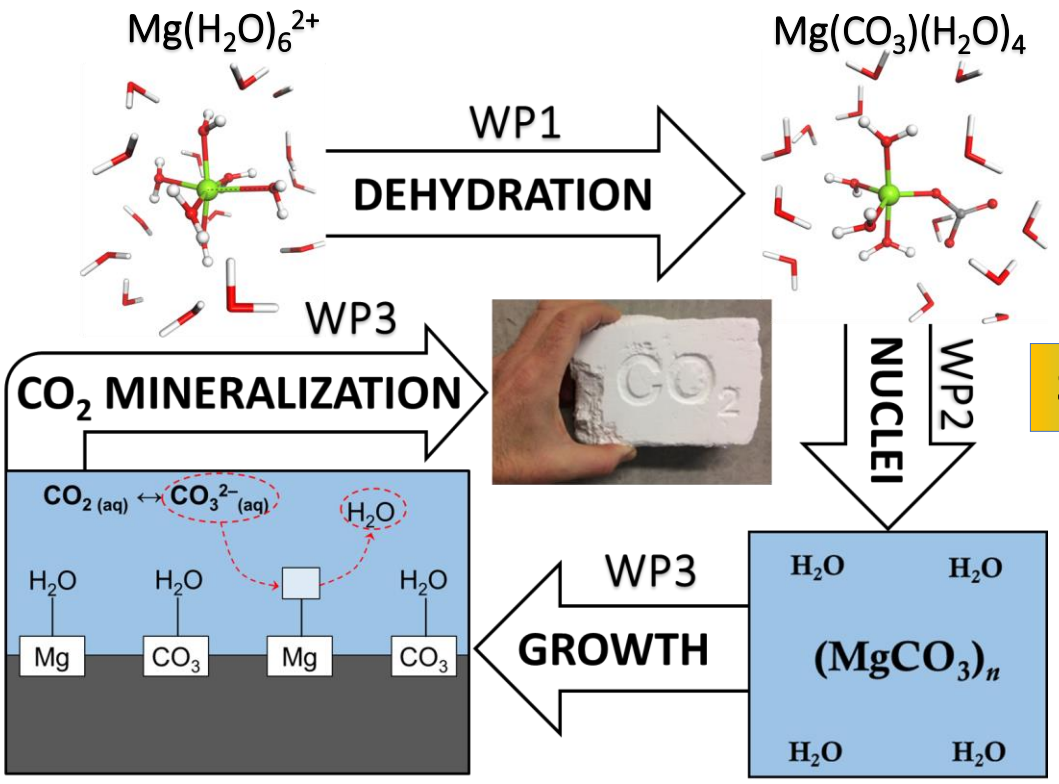


"Unravelling the fundamental mechanism that drive carbon mineralization reactions is the missing link to deploying carbon mineralization as a real-world mitigation solution to climate change"

CO_2 Utilization Priority Research Direction U5: **Accelerating Carbon Mineralization by Harnessing the Complexity of Solid-Liquid Interfaces**, in "Mission Innovation Carbon Capture, Utilization, and Storage Workshop"

The objectives of FUNMIN

INDUSTRIAL PROBLEM ⟷ **FUNMIN** ⟷ ACADEMIC EXPERTISE



SCALE-UP
WP4

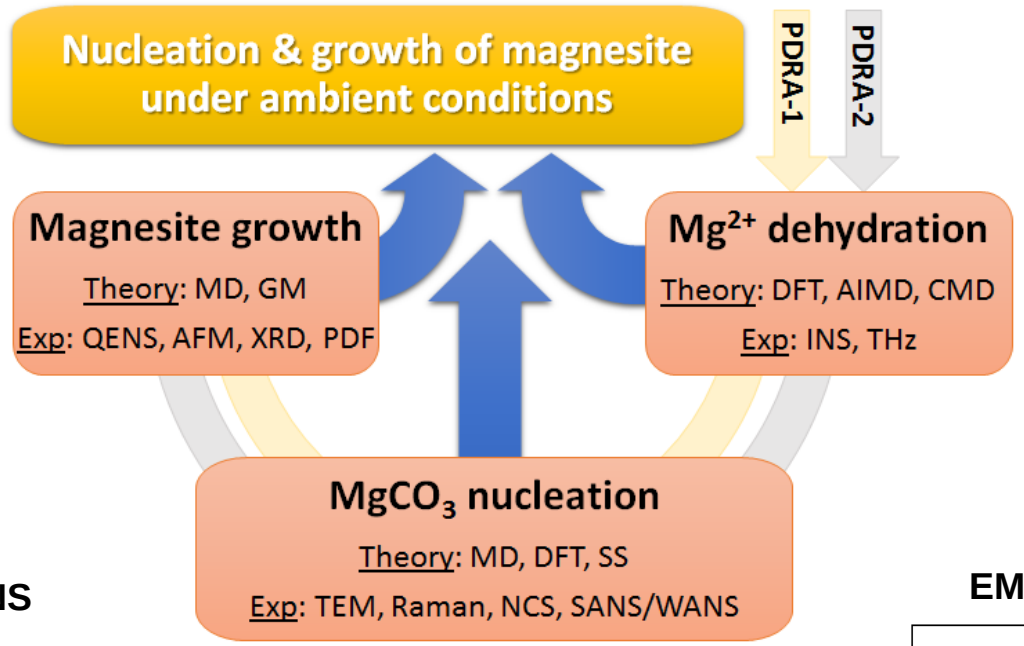
Fast-tracked optimisation of cost-effective mineralised-CO_2 materials under *mild*, *non-hazardous*, *non-toxic* conditions

Mechanism of Mg-dehydration	$MgCO_3$ nucleation pathway	Magnesite growth processes	CO_2 mineral under mild conditions

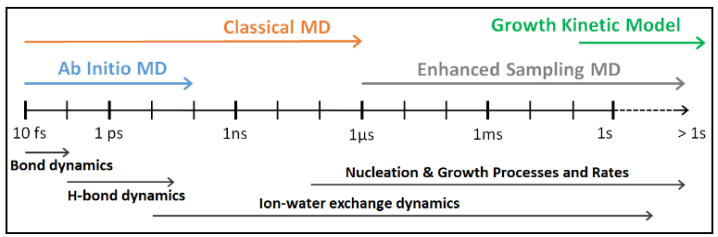
THE OBJECTIVES

The FUNMIN approach

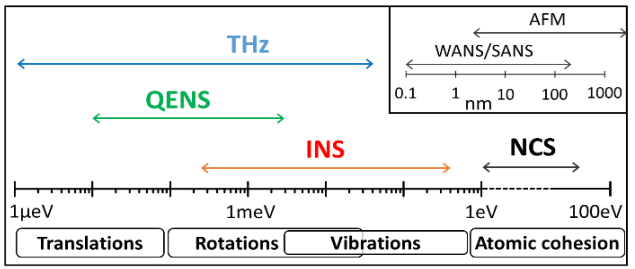
Complementary **atomistic simulations** & **spectroscopic measurements** to reveal the molecular-level processes controlling $MgCO_3$ formation: Mg-dehydration, $MgCO_3$ nucleation & growth.



THEORETICAL SIMULATIONS

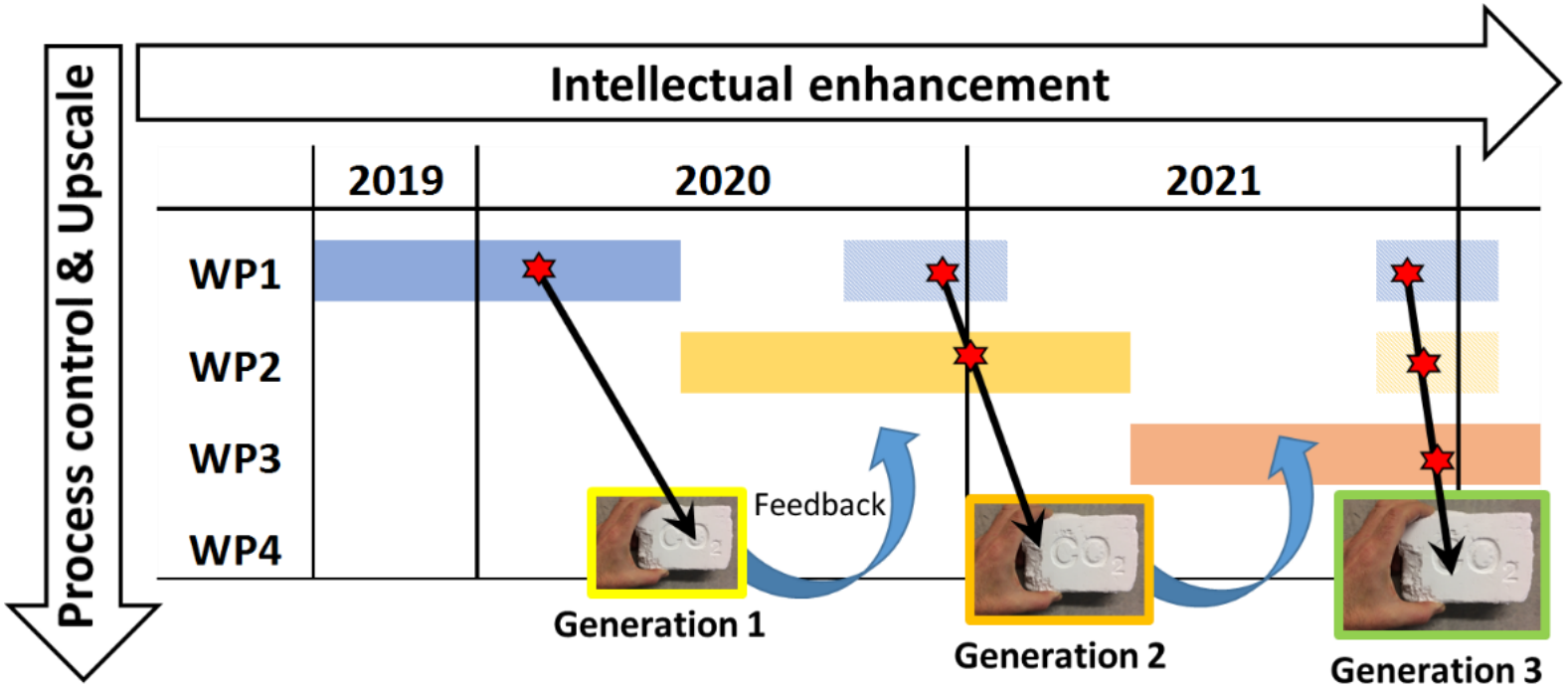


EMPIRICAL DETERMINATIONS



Project implementation

Core scientific activities (**WP1-3**) to characterize the **molecular processes** controlling magnesite crystallization; applied component (**WP4**) to **optimise** process conditions



Interaction between the scientific (**WP1-3**) and practical (**WP4**) components of the project.
WP1: Mg-dehydration; **WP2**: $MgCO_3$ nucleation; **WP3**: Magnesite Growth; **WP4**: Upscaling

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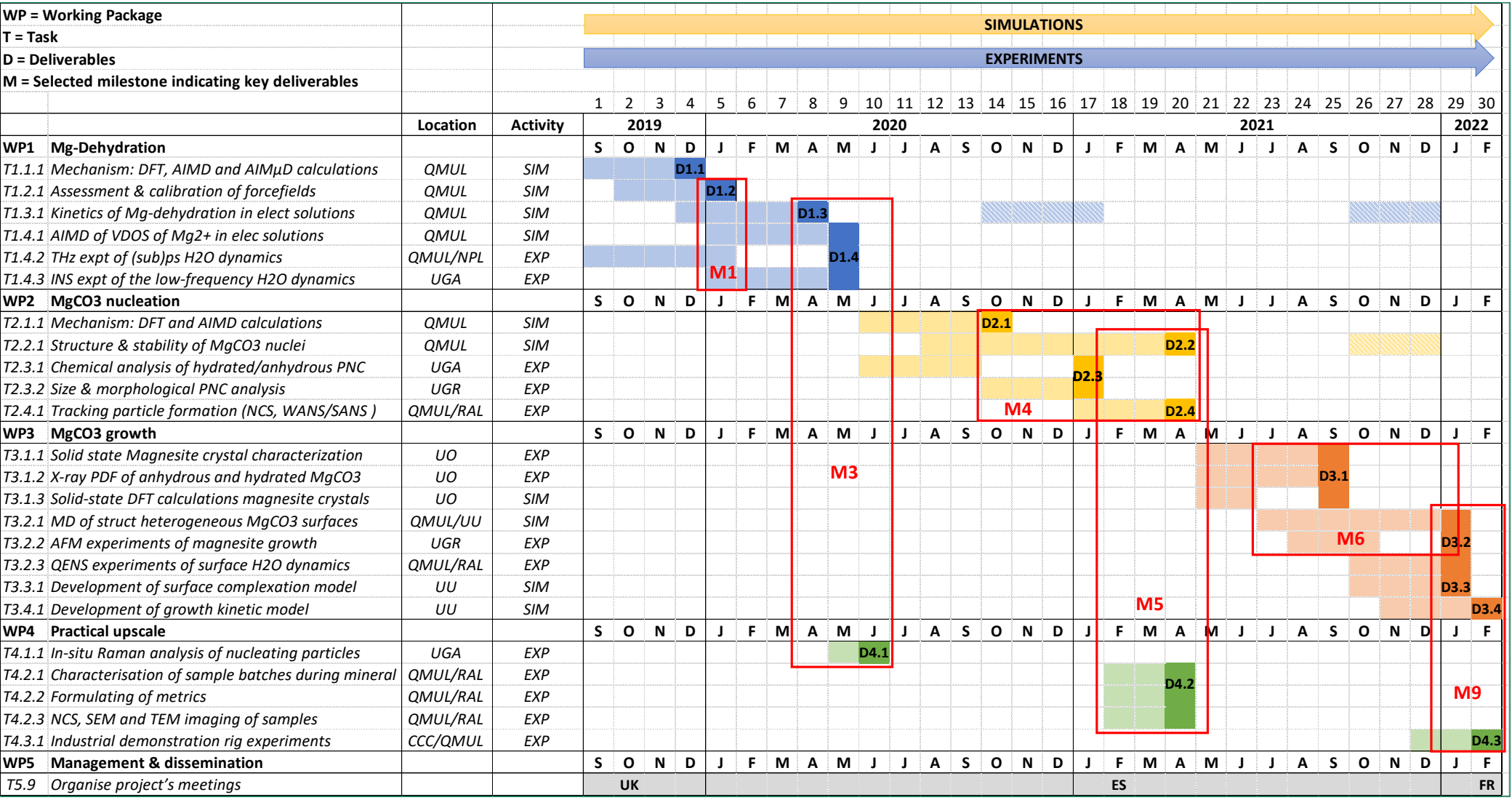
Project implementation



Project implementation

No.	Milestone Title
M1	Assessment & calibration of atomistic models
M2	First ever Neutron Compton scattering experiment for tracking $MgCO_3$ particle formation complete
M3	Effect of additives promoting Mg-dehydration, on the kinetics of crystallization of anhydrous and hydrated Mg-carbonate phases
M4	Theoretical model of $MgCO_3$ nucleation from solution developed
M5	In-situ tracking of mechanical properties & changes therein
M6	Mechanistic model of the magnesite growth in aqueous electrolyte solutions
M7	Site-specific surface complexation model for calcite developed
M8	Site-specific growth kinetic model for magnesite
M9	Factors catalysing magnesite crystallization under mild, non-hazardous, non-toxic conditions identified

WP = Working Package
T = Task
D = Deliverables
M = Selected milestone indicating key deliverables

		Location	Act
WP1	**Mg-Dehydration**		
T1.1.1	*Mechanism: DFT, AIMD and AIMµD calculations*	*QMUL*	*SI*
T1.2.1	*Assessment & calibration of forcefields*	*QMUL*	*SI*
T1.3.1	*Kinetics of Mg-dehydration in elect solutions*	*QMUL*	*SI*
T1.4.1	*AIMD of VDOS of Mg2+ in elec solutions*	*QMUL*	*SI*
T1.4.2	*THz expt of (sub)ps H2O dynamics*	*QMUL/NPL*	*E*
T1.4.3	*INS expt of the low-frequency H2O dynamics*	*UGA*	*E*
WP2	**MgCO3 nucleation**		
T2.1.1	*Mechanism: DFT and AIMD calculations*	*QMUL*	*SI*
T2.2.1	*Structure & stability of MgCO3 nuclei*	*QMUL*	*SI*
T2.3.1	*Chemical analysis of hydrated/anhydrous PNC*	*UGA*	*E*
T2.3.2	*Size & morphological PNC analysis*	*UGR*	*E*
T2.4.1	*Tracking particle formation (NCS, WANS/SANS)*	*QMUL/RAL*	*E*
WP3	**MgCO3 growth**		
T3.1.1	*Solid state Magnesite crystal characterization*	*UO*	*E*
T3.1.2	*X-ray PDF of anhydrous and hydrated MgCO3*	*UO*	*E*
T3.1.3	*Solid-state DFT calculations magnesite crystals*	*UO*	*SI*
T3.2.1	*MD of struct heterogeneous MgCO3 surfaces*	*QMUL/UU*	*SI*
T3.2.2	*AFM experiments of magnesite growth*	*UGR*	*E*
T3.2.3	*QENS experiments of surface H2O dynamics*	*QMUL/RAL*	*E*
T3.3.1	*Development of surface complexation model*	*UU*	*SI*
T3.4.1	*Development of growth kinetic model*	*UU*	*SIM*
WP4	**Practical upscale**		
T4.1.1	*In-situ Raman analysis of nucleating particles*	*UGA*	*EXP*
T4.2.1	*Characterisation of sample batches during mineral*	*QMUL/RAL*	*EXP*
T4.2.2	*Formulating of metrics*	*QMUL/RAL*	*EXP*
T4.2.3	*NCS, SEM and TEM imaging of samples*	*QMUL/RAL*	*EXP*
T4.3.1	*Industrial demonstration rig experiments*	*CCC/QMUL*	*EXP*
WP5	**Management & dissemination**		
T5.9	*Organise project's meetings*		

Task	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F
T3.4.1																		M5												D3.4
T4.1.1										D4.1																				
T4.2.1–T4.2.3																				D4.2									M9	
T4.3.1																														D4.3
T5.9		UK																ES												FR

FUNMIN Outreach plan

Dissemination audience	Dissemination Goal	Methods of Dissemination
Other Researchers working on CCUS	Understanding	Presentations and Professional Networking; Academic journals; Social media; Project's website.
Policy makers	Awareness, Understanding, Action	Formal Reports; Project meetings; Sharing research outputs.
Future Funding Organisations	Awareness, Understanding, Action	Formal reports; Social media; Sharing research outputs.
The Wider Community	Awareness	Social media; Project's website; Sharing research outputs; Outreach.

Objectives of our dissemination strategy :

- **Inform** other researchers (Chemists, Geoscientists, Industrial scientists) working on CCUS or related fields
- **Bridge** the gap between research and policy
- **Shape** funding strategy of UK and EU research councils towards CO_2 mineralization technologies
- **Interact** with the public

FUNMIN Outreach plan

- **Presentation & professional networking**
  - Presented at the FIRED-Up event (06.11.2019)
  - Press release on FUNMIN with www.consciouscomms.com
  - Kick-off meeting in London (13.12.2019)
  - Canada-UK Communities of Interest: Commercial CO_2 Capture and Use Opportunities (26.11.2019)
  - Conferences and events organised by UKCCSRC, BACG, TYC and NMUSN
- **Website & Social media**

  
  http://research.sbcs.qmul.ac.uk/d.ditommaso/funmin

  
  @FUNMIN_CO2
- **Sharing research outputs**
  - Conference papers, software, posters, presentations, reports, protocols, preprint on FUNMIN website

FUNMIN contribution to commercialisation of CO_2 mineralization

- **Scientific challenge**
  - What are the fundamental processes optimising the aqueous formation of $MgCO_3$ at low temperature in nature?
- **Technical challenge**
  - What are the process conditions that could catalyse magnesite formation under mild conditions?
- **Commercial challenge**
  - Can we develop cost-effective processes for the selective conversion of CO_2 into magnesite under mild, non-hazardous, and non-toxic conditions?
- **Provide (theory & expt) tools to the CO_2 mineralization industry**
  - To raise its impact and competitiveness

Interface between Cambridge Carbon Capture existing carbonation rig and the neutron beam facility

OBJECTIVE: reduce size and raise precision

(a)

(b)

Special Nickel-Chromium alloy for high pressure conditions

Gas handling apparatus in ISIS

Rutherford Appleton Laboratory (UK)

a) CCC's experimental set-up to observe CO_2 reaction with $Mg(OH)_2$
b) Stainless steel reaction cell for neutron measurements of heterogeneous catalyst samples (**Johnson Matthey Technol. Rev.**, 2016, 60, 132)

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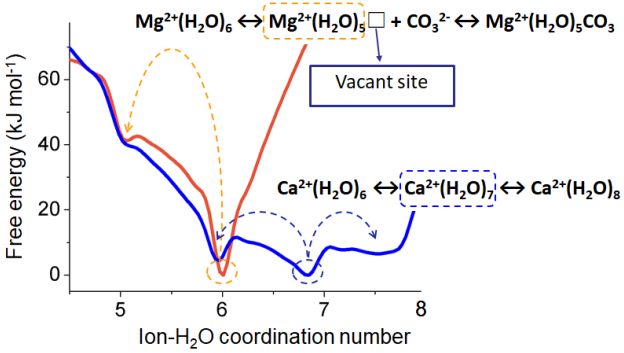
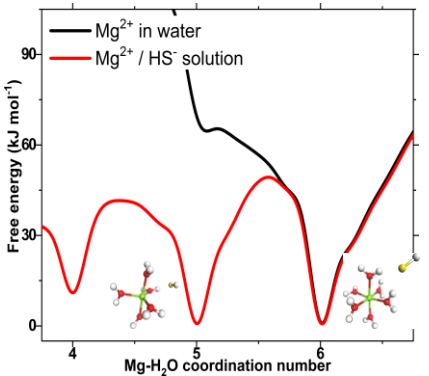
Status of FUNMIN project

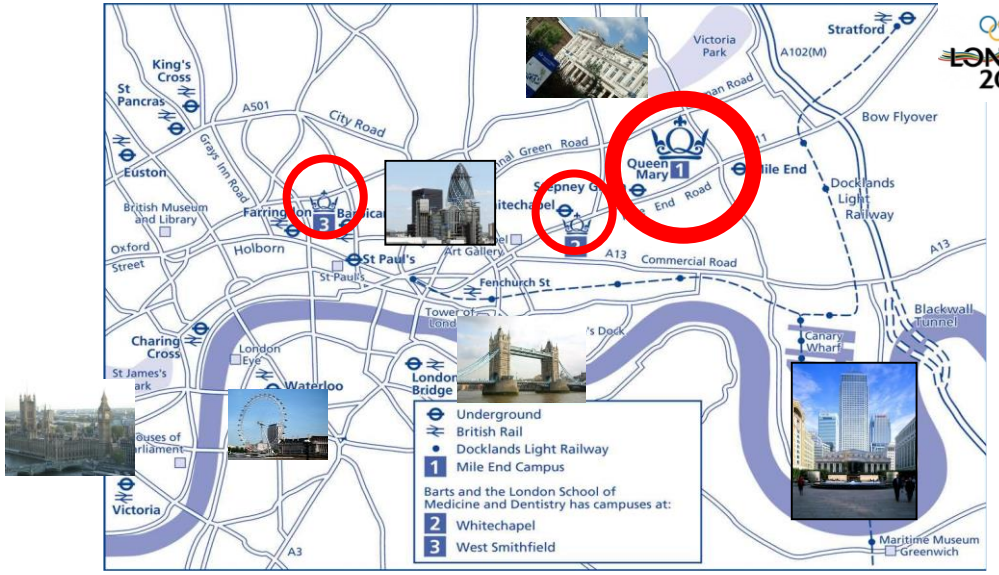
- **Contracts and Consortium agreement**
  - UK and France contracts in place. Consortium agreement signed. Spanish contract will be in place early 2020
  - QMUL hired Computational Chemist (PDRA-1) and Physical Chemist (PDRA-2)

- **First results**
  - Proposals for neutron experiments submitted to ISIS Neutron and Muon Source (UK)
  - Awarded IAA Grant to develop a flow-cell for neutron scattering measurements of CO_2 mineralisation
  - Water exchange reaction pathways around Mg^{2+} (D1.1) Dynamics of water around Mg^{2+} as a function of solution composition (D1.3)
  - Assessment & calibration of interatomic force fields (M1)





Contact us



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Acknowledgements

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http://research.sbcs.qmul.ac.uk/d.ditommaso/funmin