FUNMIN

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

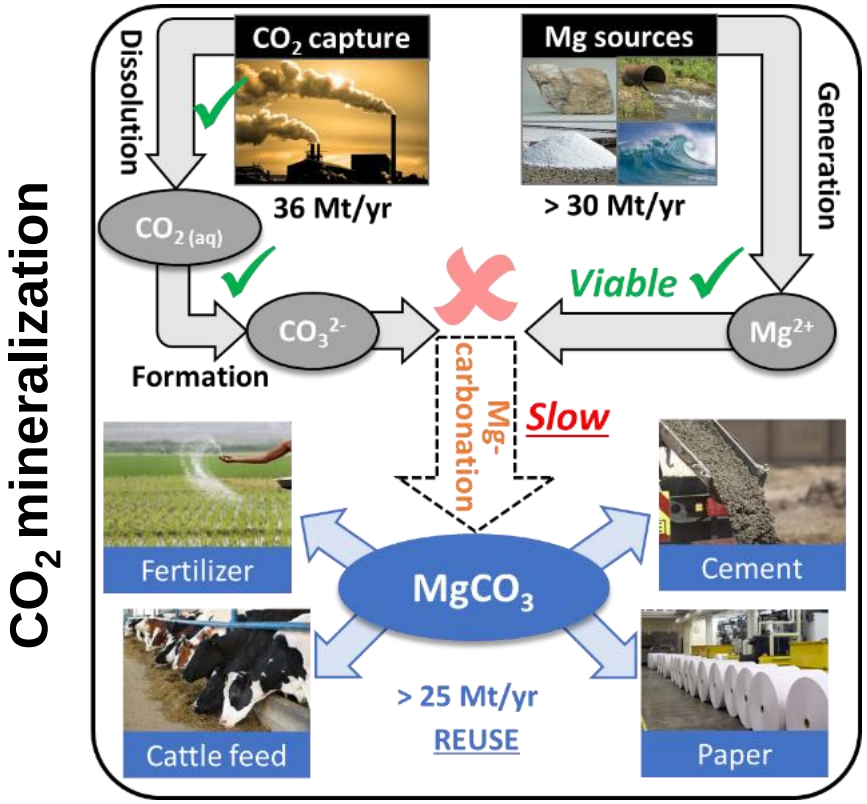
By Devis Di Tommaso, Queen Mary

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" *



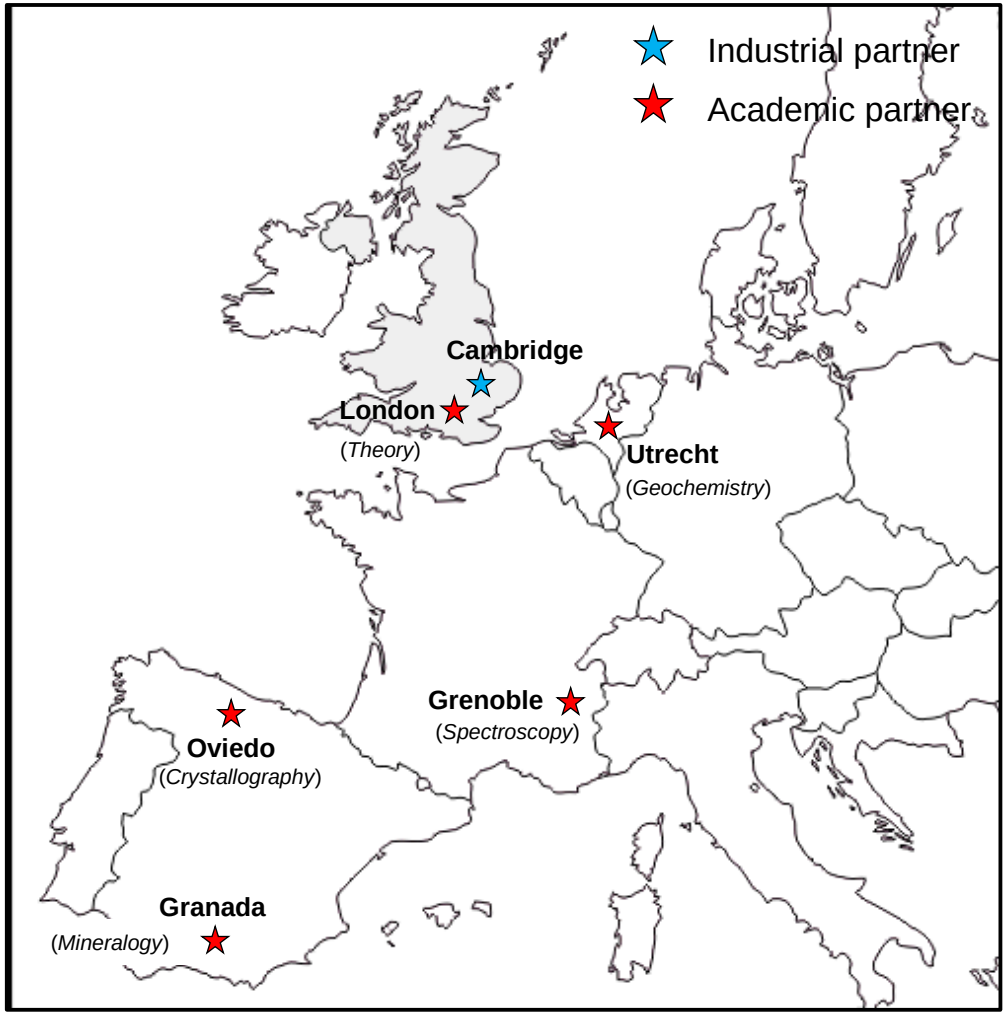
Cambridge Carbon Capture Ltd technology (**CO2LC**) to store CO_2 in mineral form ($MgCO_3$)

* 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

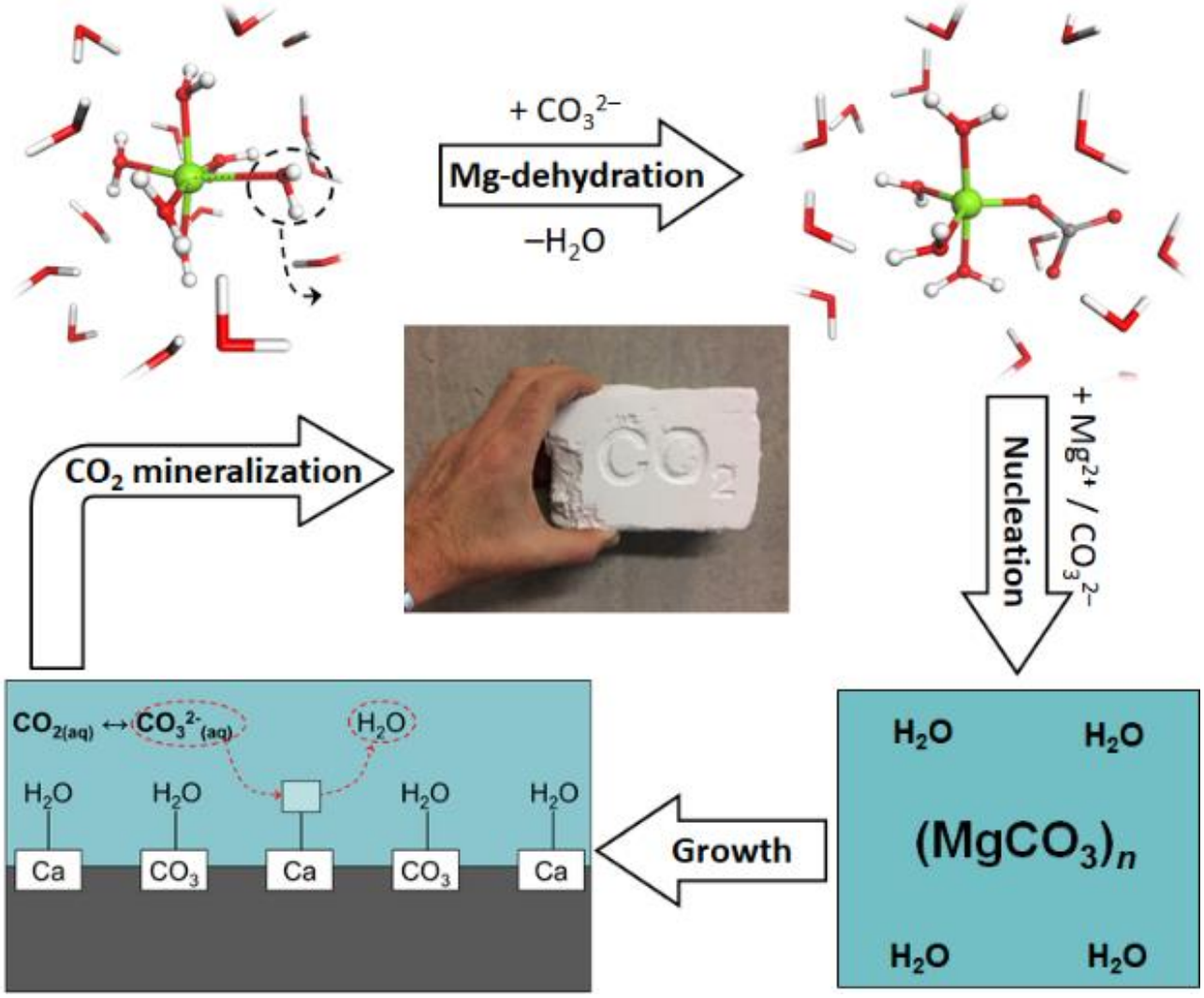
Universidad de Oviedo
Universidá d'Uviéu
University of Oviedo

UGA
Univ. Grenoble Alpes

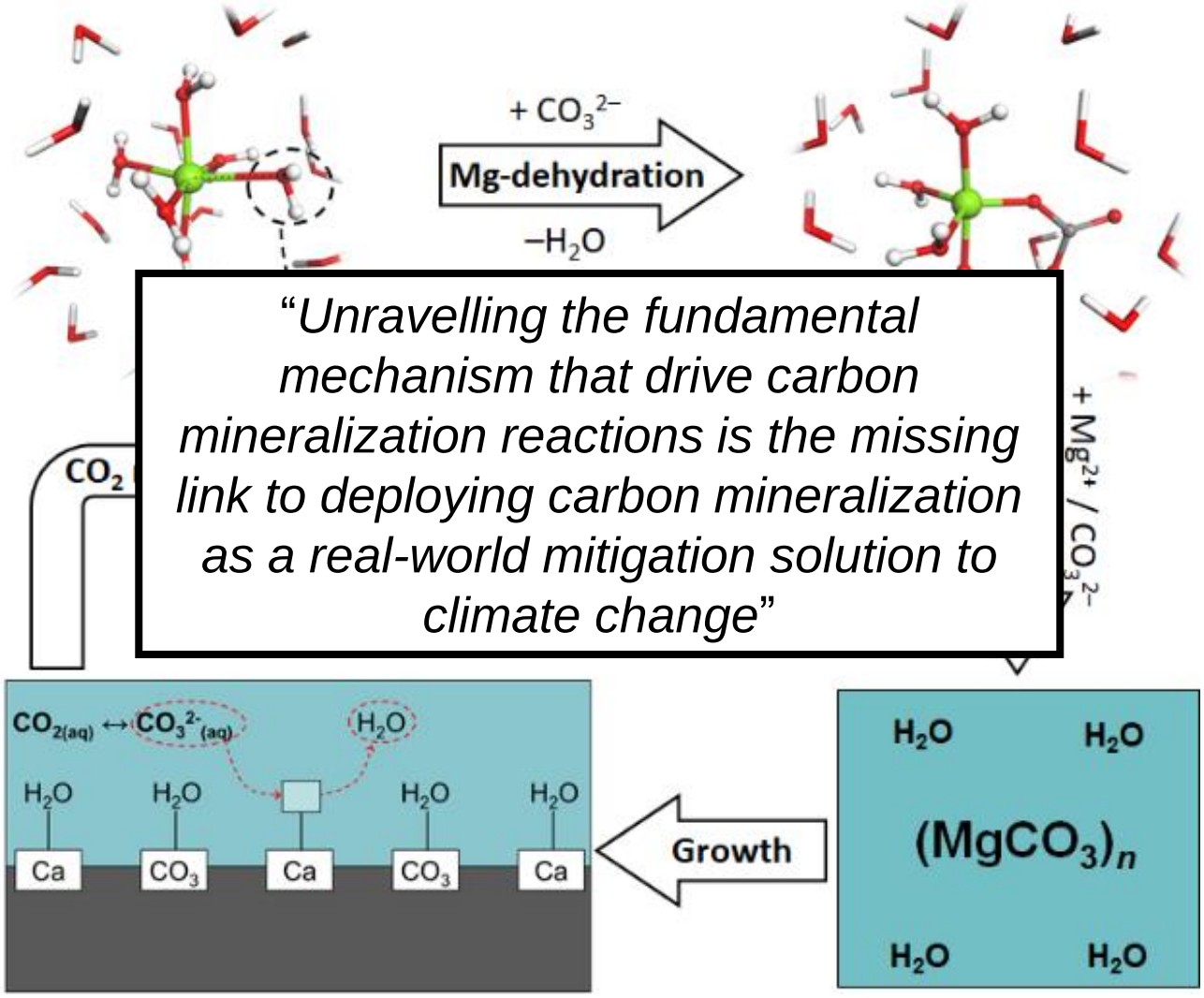
FUNMIN facts

- 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

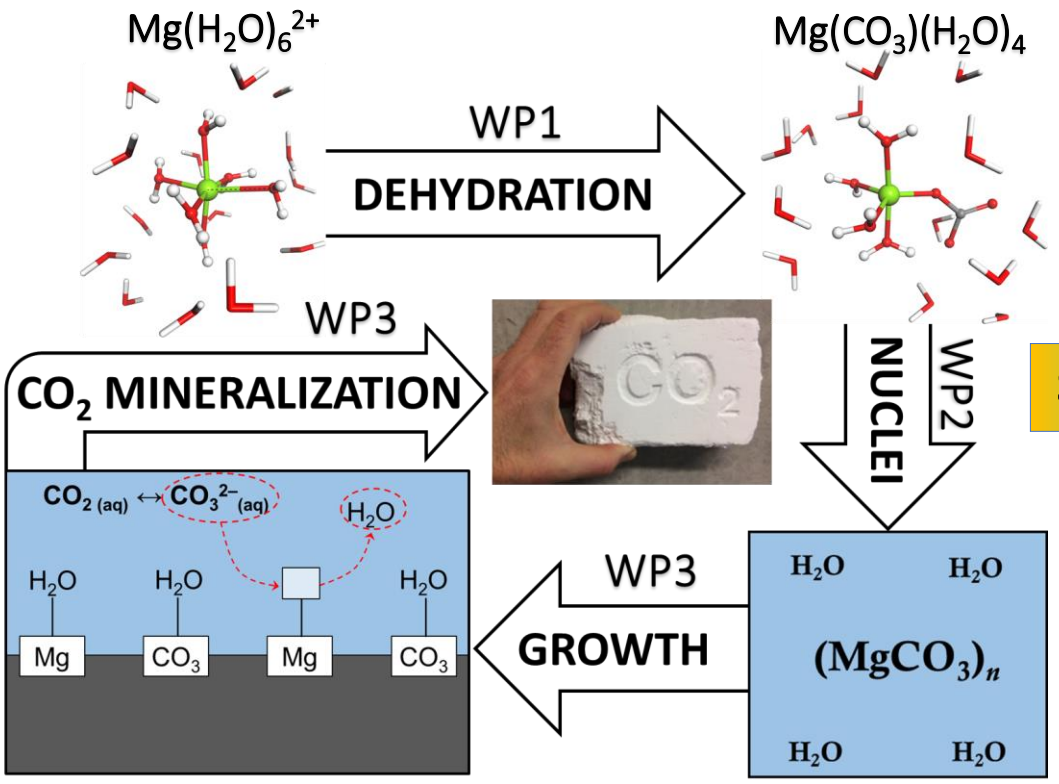


"Unravelling the fundamental mechanism that drive carbon mineralization reactions is the missing link to deploying carbon mineralization as a real-world mitigation solution to climate change"

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

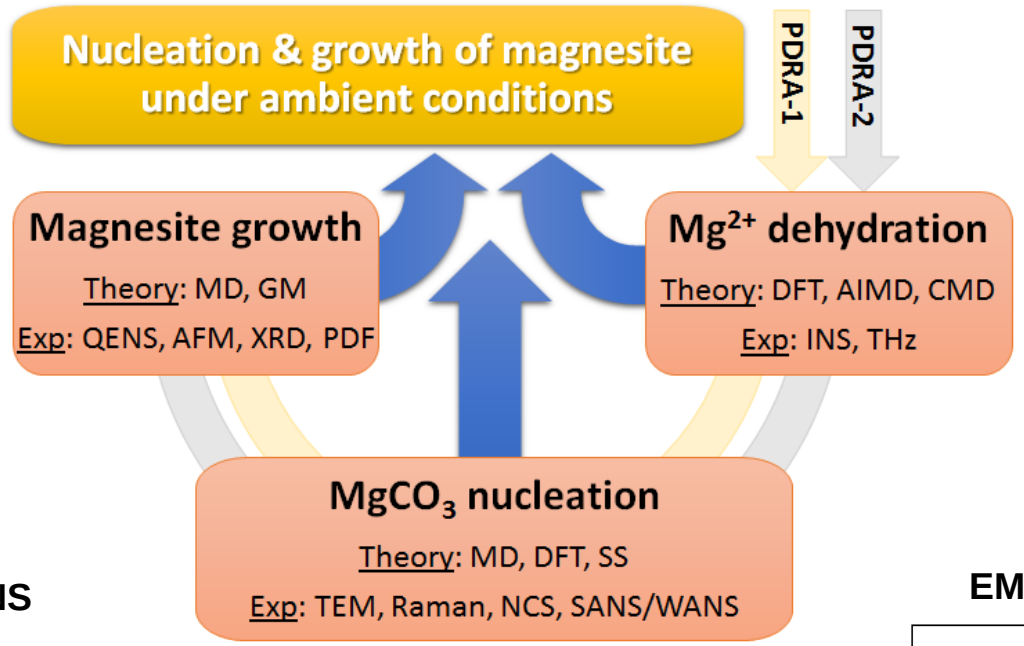
Fast-tracked optimisation of cost-effective mineralised-CO_2 materials under *mild*, *non-hazardous*, *non-toxic* conditions

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

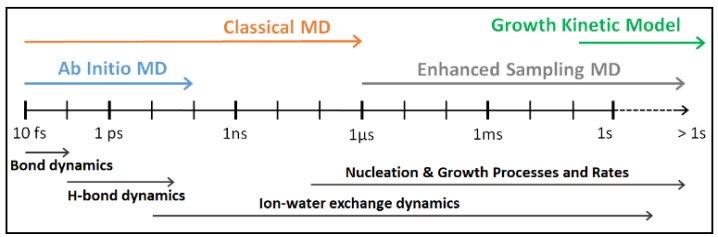
THE OBJECTIVES

The FUNMIN approach

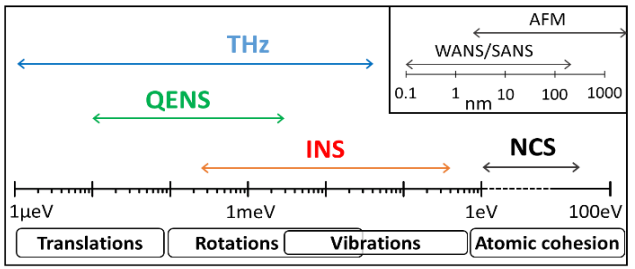
Complementary **atomistic simulations** & **spectroscopic measurements** to reveal the molecular-level processes controlling $MgCO_3$ formation: Mg-dehydration, $MgCO_3$ nucleation & growth.



THEORETICAL SIMULATIONS

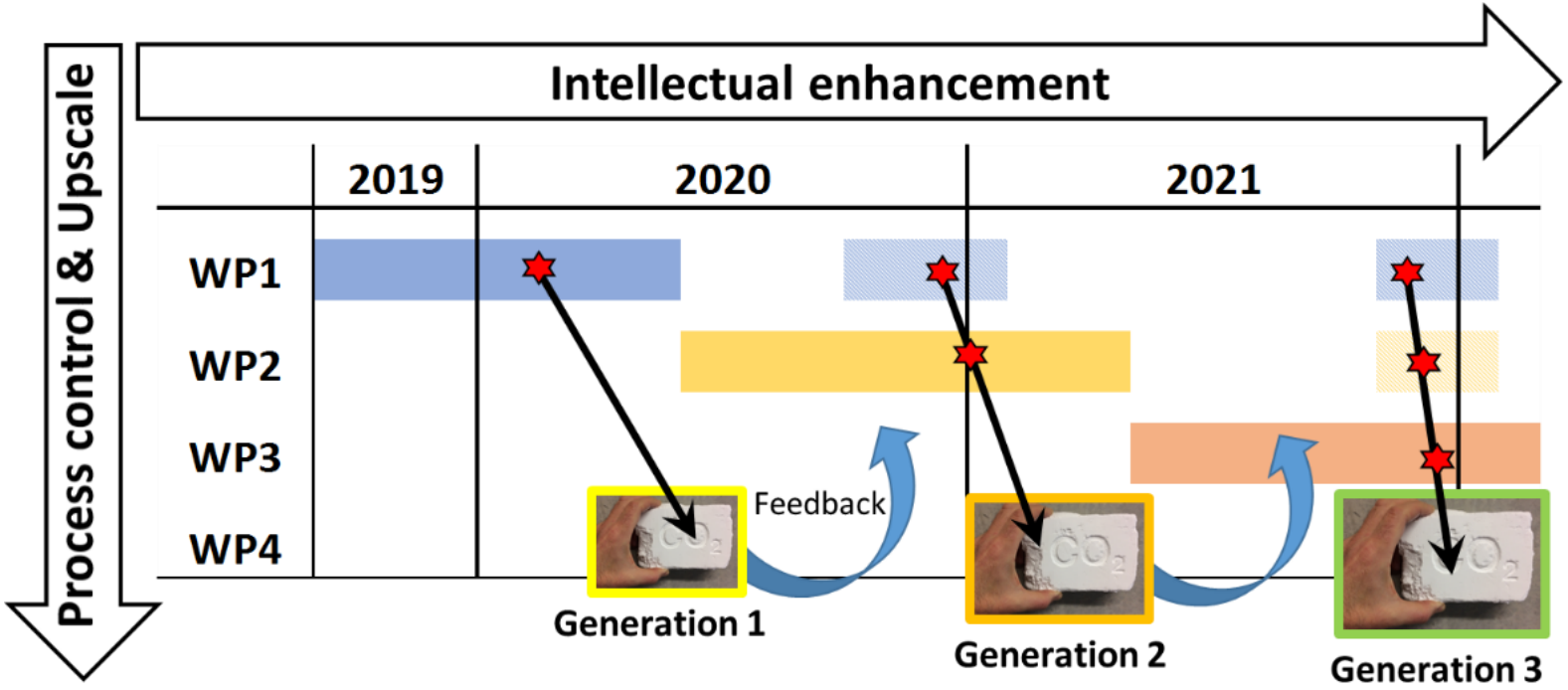


EMPIRICAL DETERMINATIONS



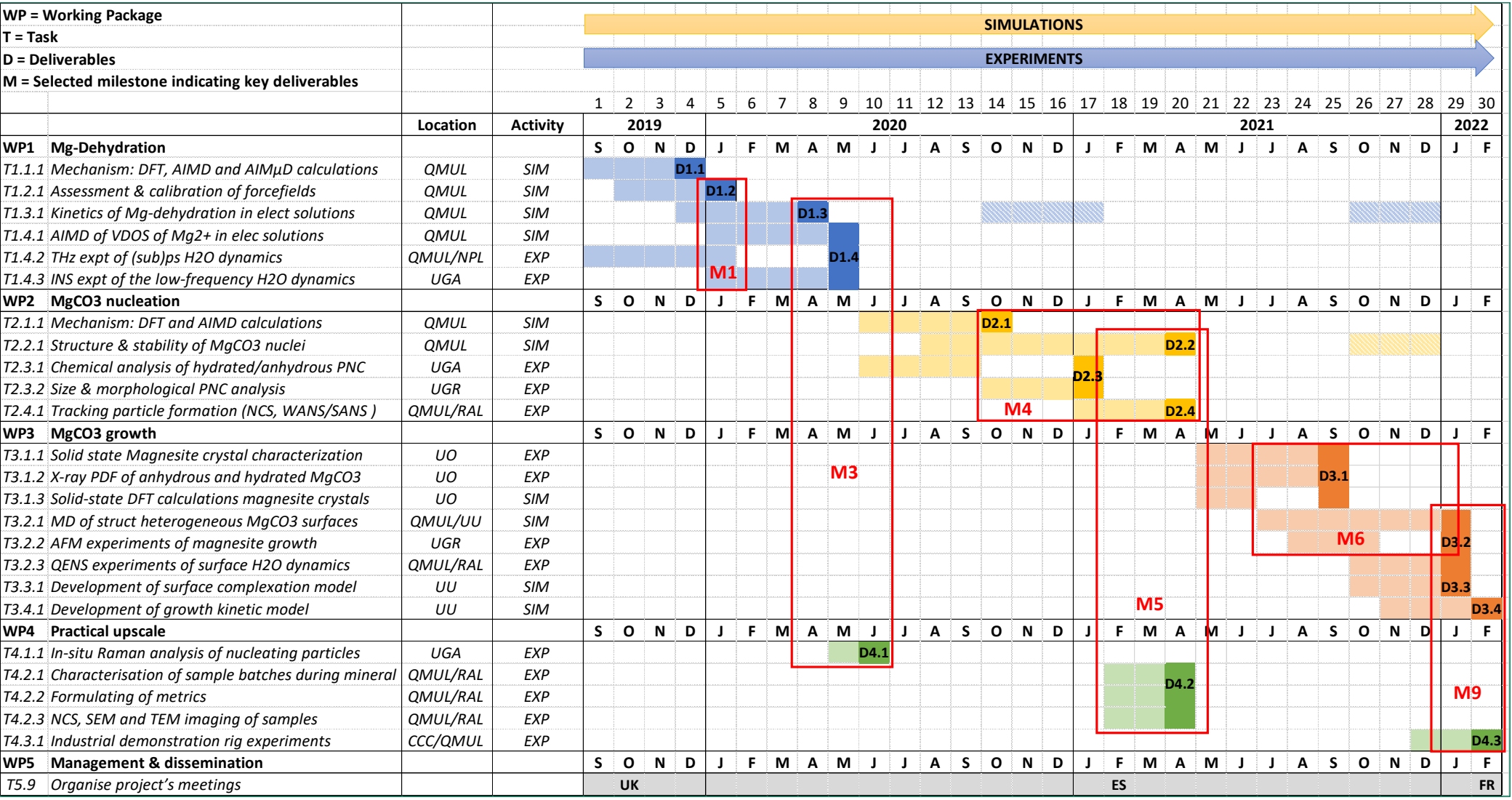
Project implementation

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

Project implementation



Queen Mary University of London

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

				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
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*	*EI*																														
T1.4.3	*INS expt of the low-frequency H2O dynamics*	*UGA*	*EI*																														
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*	*EI*																														
T2.3.2	*Size & morphological PNC analysis*	*UGR*	*EI*																														
T2.4.1	*Tracking particle formation (NCS, WANS/SANS)*	*QMUL/RAL*	*EI*																														
WP3	**MgCO3 growth**																																
T3.1.1	*Solid state Magnesite crystal characterization*	*UO*	*EI*																														
T3.1.2	*X-ray PDF of anhydrous and hydrated MgCO3*	*UO*	*EI*																														
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*	*EI*																														
T3.2.3	*QENS experiments of surface H2O dynamics*	*QMUL/RAL*	*EI*																														
T3.3.1	*Development of surface complexation model*	*UU*	*SI*																														
T3.4.1	*Development of growth kinetic model*	*UU*	*SIM*																				M5										D3.4
WP4	**Practical upscale**																																
T4.1.1	*In-situ Raman analysis of nucleating particles*	*UGA*	*EXP*										D4.1																				
T4.2.1	*Characterisation of sample batches during mineral*	*QMUL/RAL*	*EXP*																					D4.2									
T4.2.2	*Formulating of metrics*	*QMUL/RAL*	*EXP*																													M9	
T4.2.3	*NCS, SEM and TEM imaging of samples*	*QMUL/RAL*	*EXP*																														
T4.3.1	*Industrial demonstration rig experiments*	*CCC/QMUL*	*EXP*																													D4.3	
WP5	**Management & dissemination**			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
T5.9	*Organise project's meetings*				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

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)

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

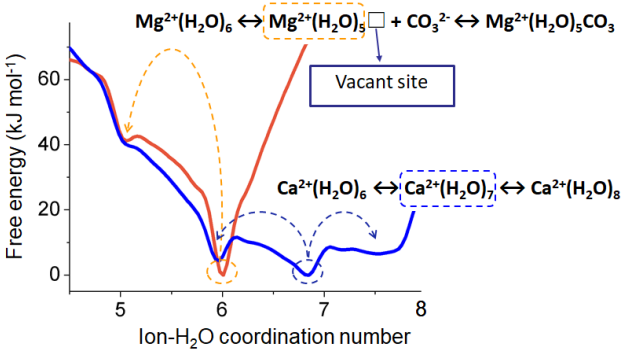
Rutherford Appleton Laboratory (UK)

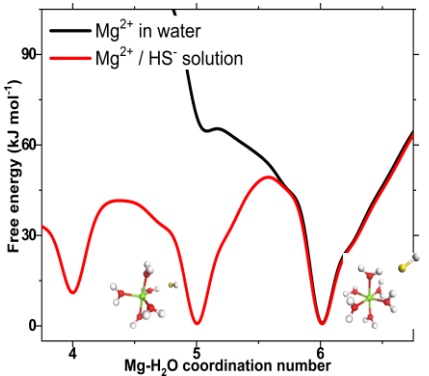
a) CCC's experimental set-up to observe CO_2 reaction with $Mg(OH)_2$
b) Stainless steel reaction cell for neutron measurements of heterogeneous catalyst samples (**Johnson Matthey Technol. Rev.**, 2016, 60, 132)

Status of FUNMIN project

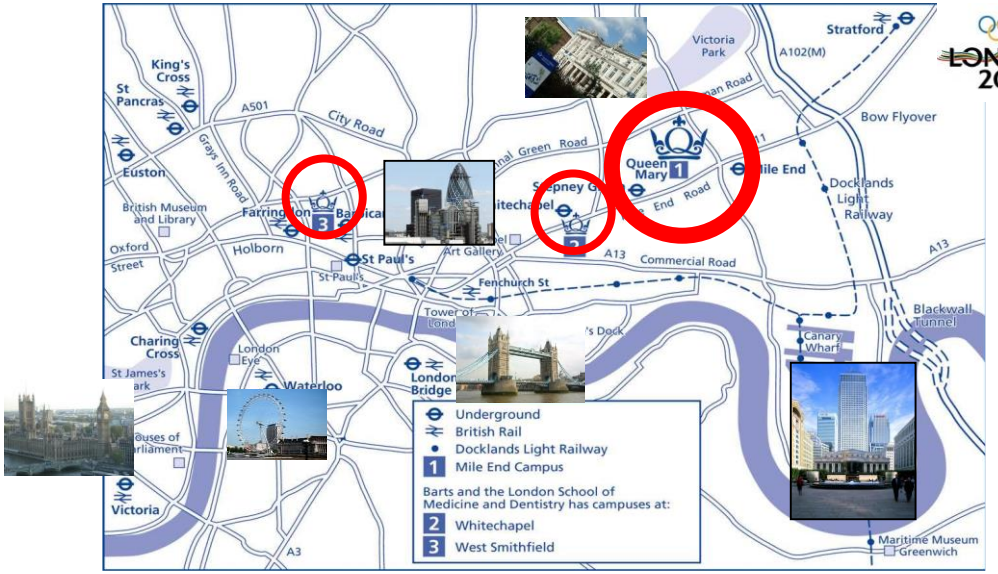
- **Contracts and Consortium agreement**
  - UK and France contracts in place. Consortium agreement signed. Spanish contract will be in place early 2020
  - QMUL hired Computational Chemist (PDRA-1) and Physical Chemist (PDRA-2)

- **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



Queen Mary, London

Queen Mary University of London

Department of Chemistry
Faculty of Science and Engineering
Mile End Road
London E1 4NS

Devis Di Tommaso

FUNMIN Project Coordinator
d.ditommaso@qmul.ac.uk

Acknowledgements

This project has been subsidized through ACT (EC Project no. 691712), by BEIS (UK), ADEME (FR), MINECO-AEI (ES)

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