FUNMIN

<u>Fun</u>damental Studies of <u>Min</u>eral Carbonation with Application to CO₂ Utilisation

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CO₂ Mineralization

Mineralization of **carbon dioxide** represents a principal raw material feedstock for carbonate-based materials, revenues of which are expected to reach \$1 trillion/yr. by 2030 (Mission Innovation, 2017)



The Challenge: CO₂ sequestration via aqueous formation of

The Consortium

World expertise in mineralization guiding Industrial technologists to permanently mineralise CO₂

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



Ca Queen Mary University of London

Cambridge Carbon Capture





magnesite (MgCO₃) is a promising carbon capture, utilization and storage technology, albeit limited by slow precipitation rates



UICA Univ. Grenoble Alpes

Overall Aims & Objectives

The aim of **FUNMIN** is to conduct the world's most evolved *simulations* & *empirical* determinations worldwide of the molecular events surrounding MgCO₃ formation (**WP1-3**), to catalytically scale-up CO₂ mineralisation (**WP4**)

Outcomes & Impact

Mechanisms of magnesite nucleation, as well as resolving the role of solution composition and surface nano-topography on crystallization kinetics; this will **Impact** CO₂ mineralization by identifying conditions that facilitate MgCO₃ fomation



Atomistic simulations & spectroscopic techniques to reveal the processes controlling $MgCO_3$ formation: Mg-dehydration, $MgCO_3$ nucleation & growth.



Theory: density functional theory (DFT), ab initio (AIMD) & classical MD (CMD) molecular dynamics, enhanced sampling (ES), structure searching (SS), geochemical modelling (GM)

Expt: quasi-elastic (QENS), Compton (NCS), wide and small angle (WANS/SANS) neutron scattering, X-ray diffraction (XRD) and pair distribution function (PDF), atomic force (AFM) and transmission electron (TEM) microscopy, Raman and THz

Methodology & Implementation of the Project

WP = Working Package														S	SIMU	JLAT		S														
T = Task																																K
D = Deliverables															E	EXPE	RIM	IENT	S		;								Ļ			
M = Selected milestone indicating key deliverables																																·
			1	2	3	4	5	6	7	8	9 2	10	11	12	13 1	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	Location	Activity		20:	19							202	0								{	}	:	20	21						20	22
WP1 Mg-Dehydration			S	0	Ν	D	J	F	Μ	Α	Μ	J	J	Α	S	0	Ν	D	J	F	Μ	Α	Μ	J	J	Α	S	0	N	D	J	F
T1.1.1 Mechanism: DFT, AIMD and AIMµD calculations	QMUL	SIM			C	01.1																					ļļ					
T1.2.1 Assessment & calibration of forcefields	QMUL	SIM				D	1.2																									
T1.3.1 Kinetics of Mg-dehydration in elect solutions	QMUL	SIM							C	01.3																						ļ
T1.4.1 AIMD of VDOS of Mg2+ in elec solutions	QMUL	SIM																														
T1.4.2 THz expt of (sub)ps H2O dynamics	QMUL/NPL	EXP									D1.4																					
T1.4.3 INS expt of the low-frequency H2O dynamics	UGA	EXP					VI1																									[
WP2 MgCO3 nucleation			S	0	Ν	D	J	F	м	Α	М	J	J	Α	S	0	Ν	D	J	F	Μ	Α	М	J	J	Α	S	0	Ν	D	J	F
T2.1.1 Mechanism: DFT and AIMD calculations	QMUL	SIM													D	<mark>)2.1</mark>																
T2.2.1 Structure & stability of MgCO3 nuclei	QMUL	SIM																				D2.2										
T2.3.1 Chemical analysis of hydrated/anhydrous PNC	UGA	EXP																														
T2.3.2 Size & morphological PNC analysis	UGR	EXP																	UZ.5													
T2.4.1 Tracking particle formation (NCS, WANS/SANS)	QMUL/RAL	EXP														Μ	14					D2.4										
WP3 MgCO3 growth			S	0	Ν	D	J	F	м	Α	Μ	J	J	Α	S	0	Ν	D	J	F	Μ	Α	М	J	J	Α	S	0	Ν	D	J	F
T3.1.1 Solid state Magnesite crystal characterization	UO	EXP																														_
T3.1.2 X-ray PDF of anhydrous and hydrated MgCO3	UO	EXP									M3																D3.1					
T3.1.3 Solid-state DFT calculations magnesite crystals	UO	SIM																														1
T3.2.1 MD of struct heterogeneous MgCO3 surfaces	QMUL/UU	SIM																														1
T3.2.2 AFM experiments of magnesite growth	UGR	EXP																									M	16		ſ	D3.2	
T3.2.3 QENS experiments of surface H2O dynamics	QMUL/RAL	EXP																						•								
T3.3.1 Development of surface complexation model	UU	SIM																												ſ	D3.3	
T3.4.1 Development of growth kinetic model	UU	SIM																			M5											D3
WP4 Practical upscale			S	0	Ν	D	J	F	м	Α	м	J	J	Α	S	0	Ν	D	J	F	М	Α	м	J	J	Α	S	0	Ν	D	J	F
T4.1.1 In-situ Raman analysis of nucleating particles	UGA	EXP									D	4.1																				
T4.2.1 Characterisation of sample batches durina mineral	OMUL/RAL	EXP																														
T4.2.2 Formulating of metrics	QMUL/RAL	EXP																				D4.2									Μ	9
T4.2.3 NCS, SEM and TEM imaaina of samples	QMUL/RAL	EXP																														
T4.3.1 Industrial demonstration ria experiments	ссс/оми	EXP																	Ŀ					1								D4
WP5 Management & dissemination			S	0	N	D	J	F	м	Α	м	J	J	Α	S	0	N	D	J	F	М	Α	м	J	J	Α	S	0	N	D	J	F
T5 9 Organise project's meetings			-	<u>-</u>		-		-				-	-		-	-		-	-	FS				-	-		-	-		Ť	-	F