# Nanoengineered C-S-H Using Biomimetic Molecules for Enhanced Functionality

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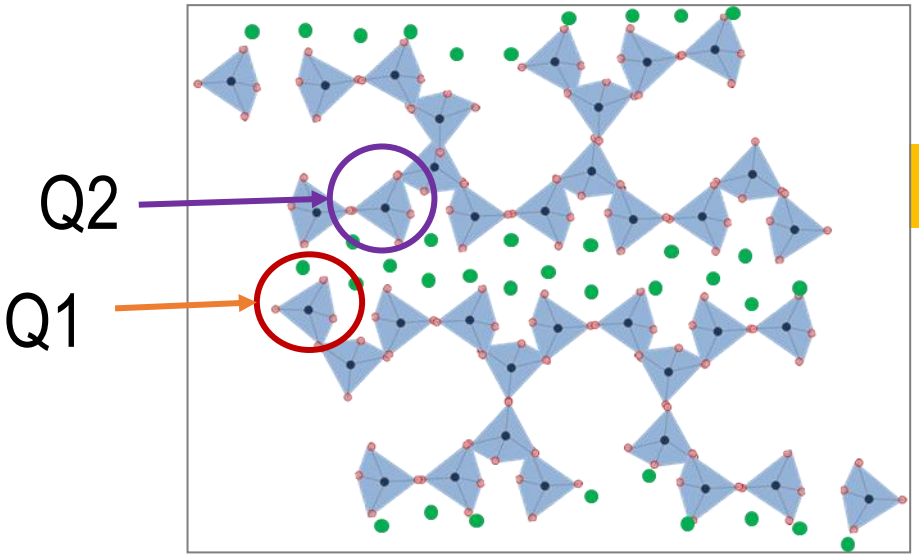
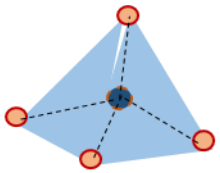
# Carbonation Degradation of C-S-H



*Calcium Silicate Hydrate (C-S-H)* $+ CO_2 + H_2O \rightarrow SiO_2.H_2O + CaCO_3$




C-S-H



$SiO_4^{-4}$ Units

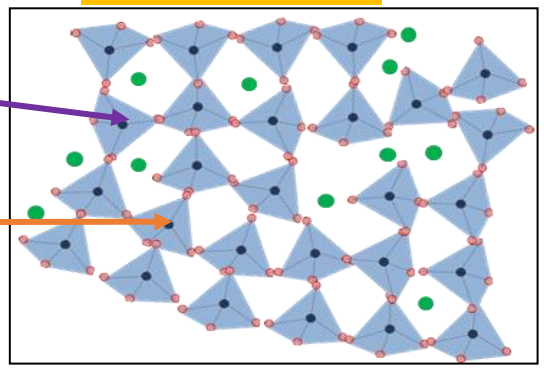
$Ca^{+2}$

\+

$H^+ + HCO_3^-$

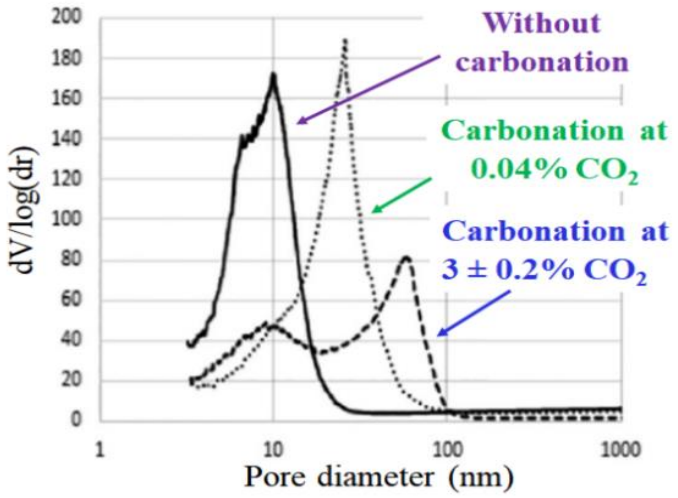
Carbonation

Silica gel



# Carbonation Degradation of C-S-H

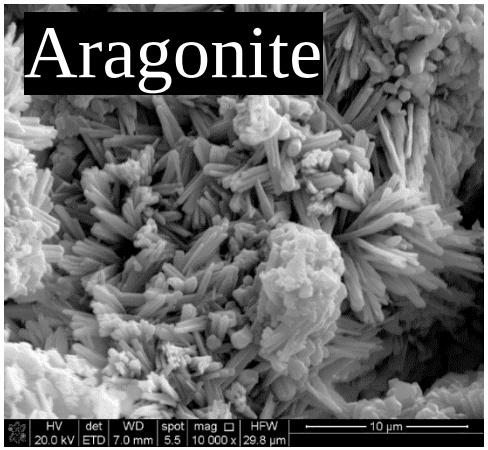
- Around 0.04% of $CO_2$ present in atmosphere
- C-S-H carbonation cause shrinkage, reduced pH, and increased critical pore size



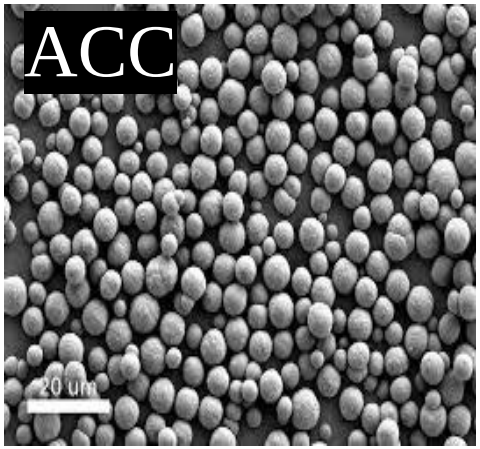

- A problem for
  - *Ca-rich Alkali activated material*
  - *Concrete with high volume of SCMs*

*Carbonation induced corrosion*

# More about $CaCO_3$

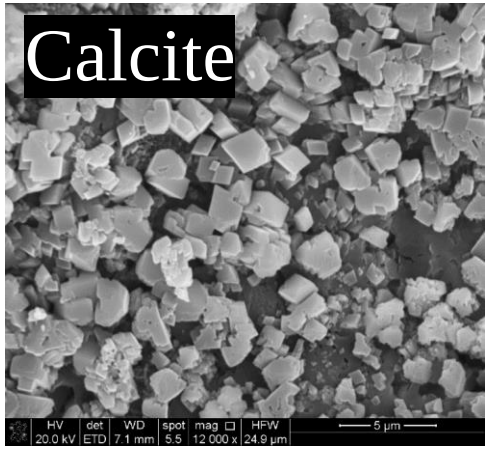






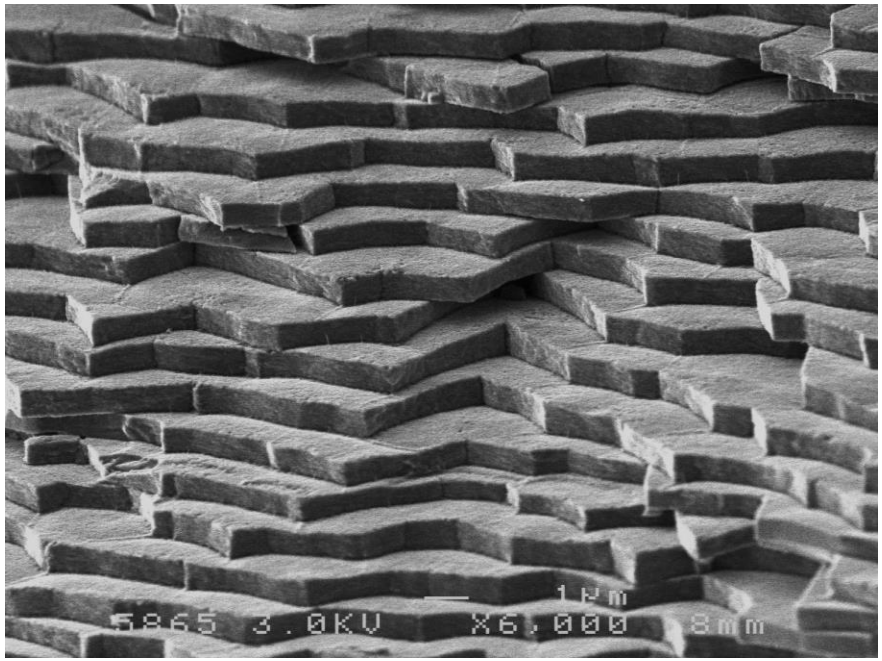

Can reduce carbonation extent

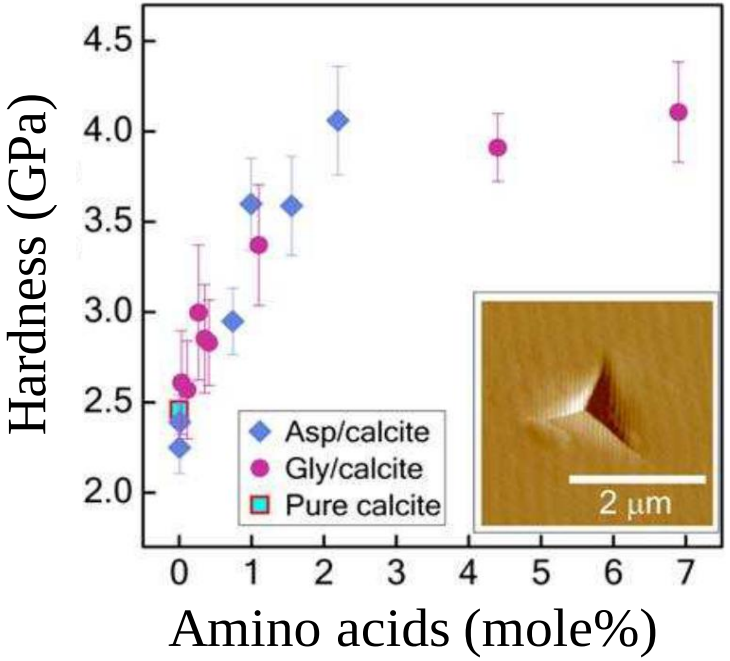
- Calcite, Aragonite, Vaterite and ACC
- Solubility and hardness of polymorphs are different
- Exact polymorphs depends on pH, $CO_2$ concentration, RH, etc.




*How can we control $CaCO_3$ crystallization?*

# Role Biomimetic molecules



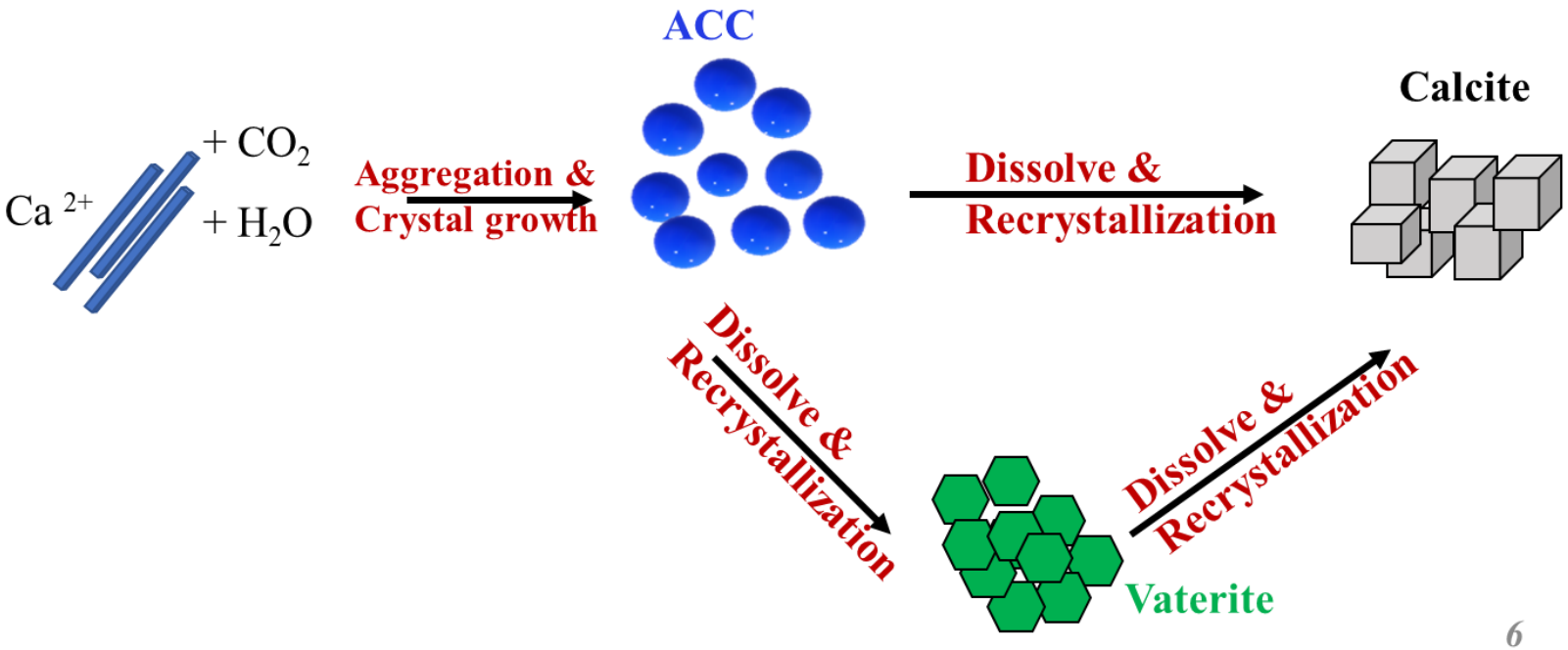




*Kim et al. Nature Materials 2016*

- Some specific biochemicals can affect the crystallization of $CaCO_3$
- This process results in the formation of 'organic-inorganic' hybrid material with superior mechanical performance.

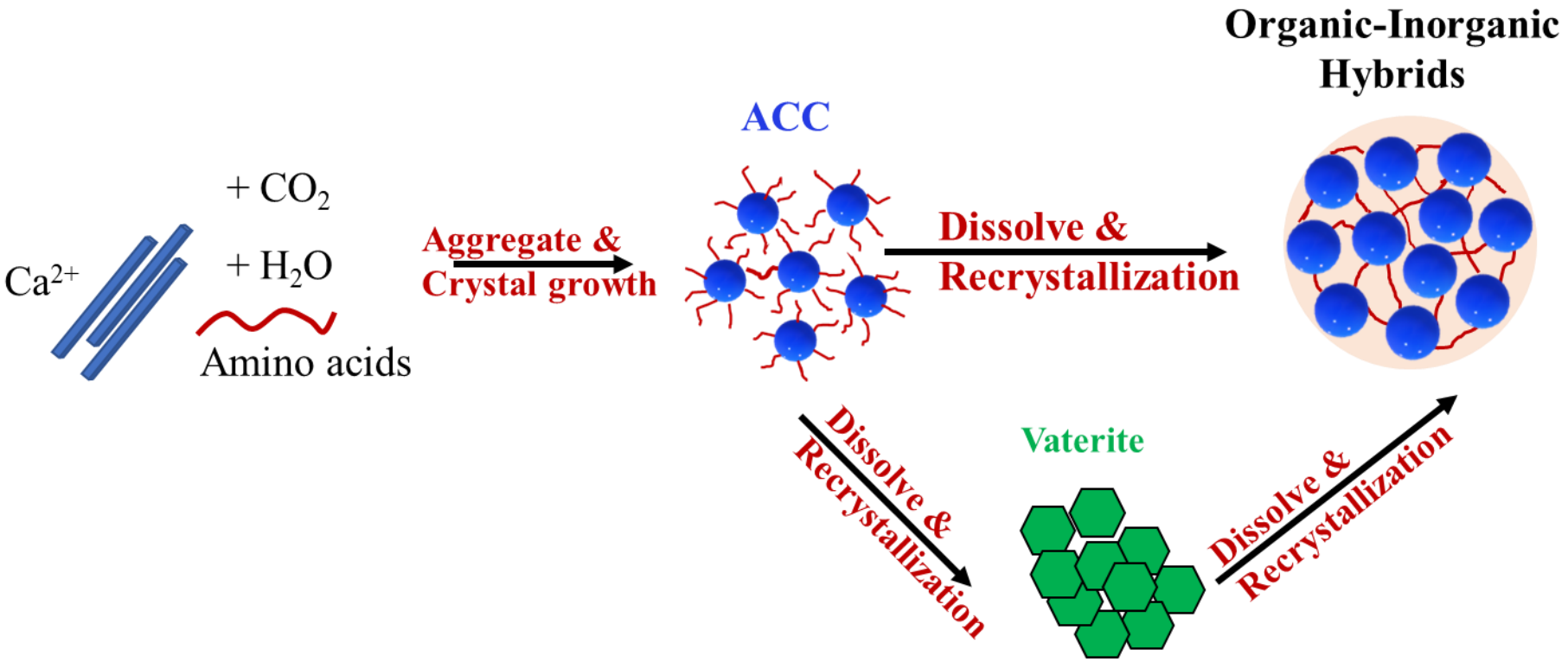
# More about $CaCO_3$

## $CaCO_3$ crystallization without biomimetic molecules



# More about $CaCO_3$

## $CaCO_3$ crystallization with biomimetic molecules

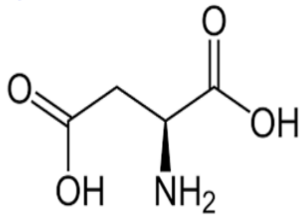


# Research Goal

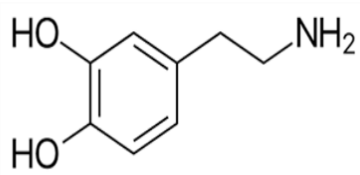
Applications of **biomimetic molecules** to prevent the deterioration of calcium silicate hydrate (C-S-H) during carbonation

# Experimental Setup

- Biomimetic molecules

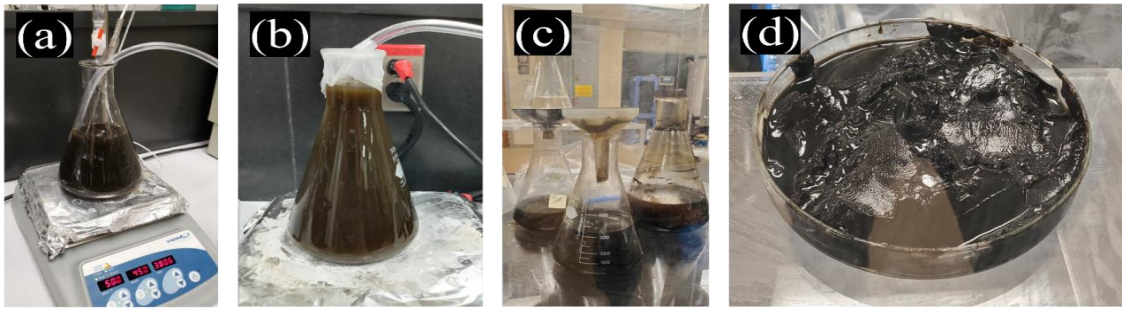



L-aspartic acid




Dopamine

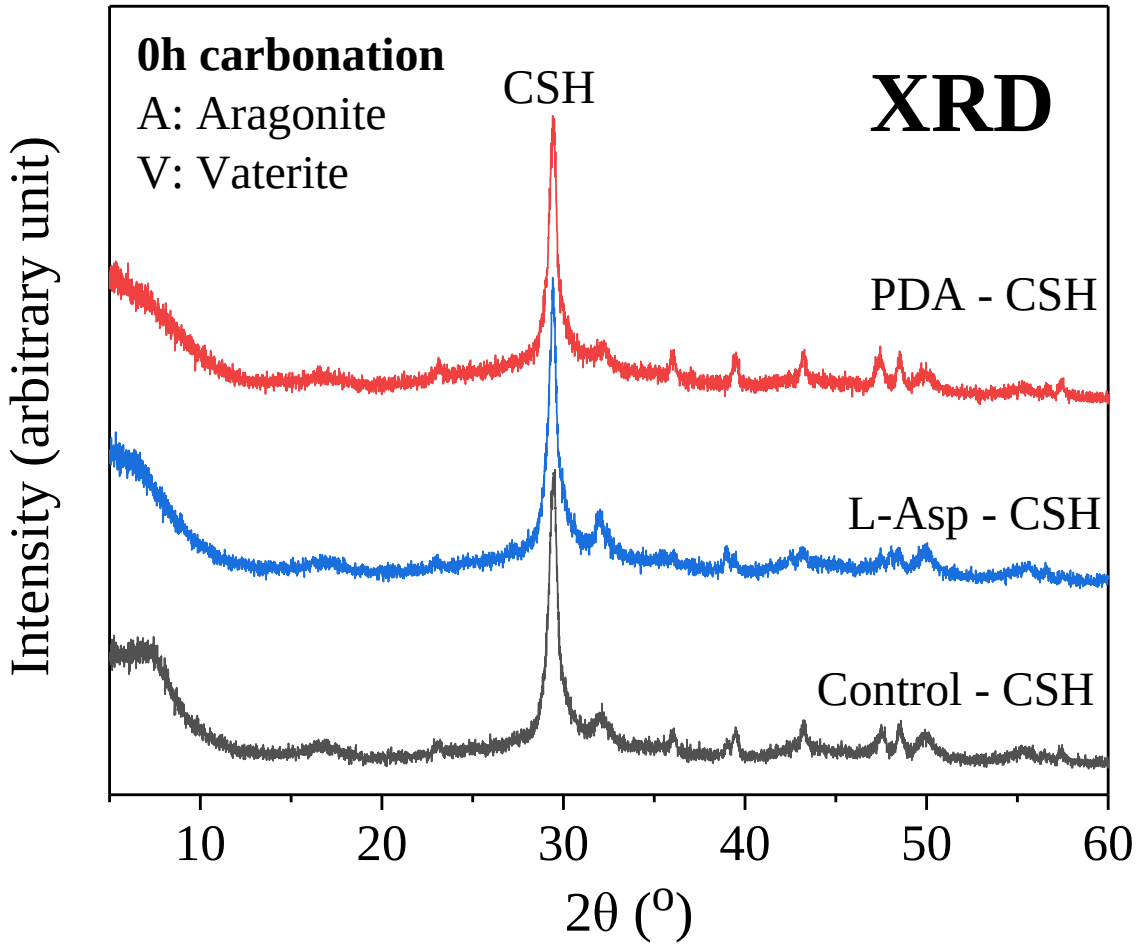
- C-S-H synthesis (Ca/Si ratio of 1.5)




- Carbonation at 4% $CO_2$ environment

# Findings

# Characteristics of synthesized C-S-H




## XRF

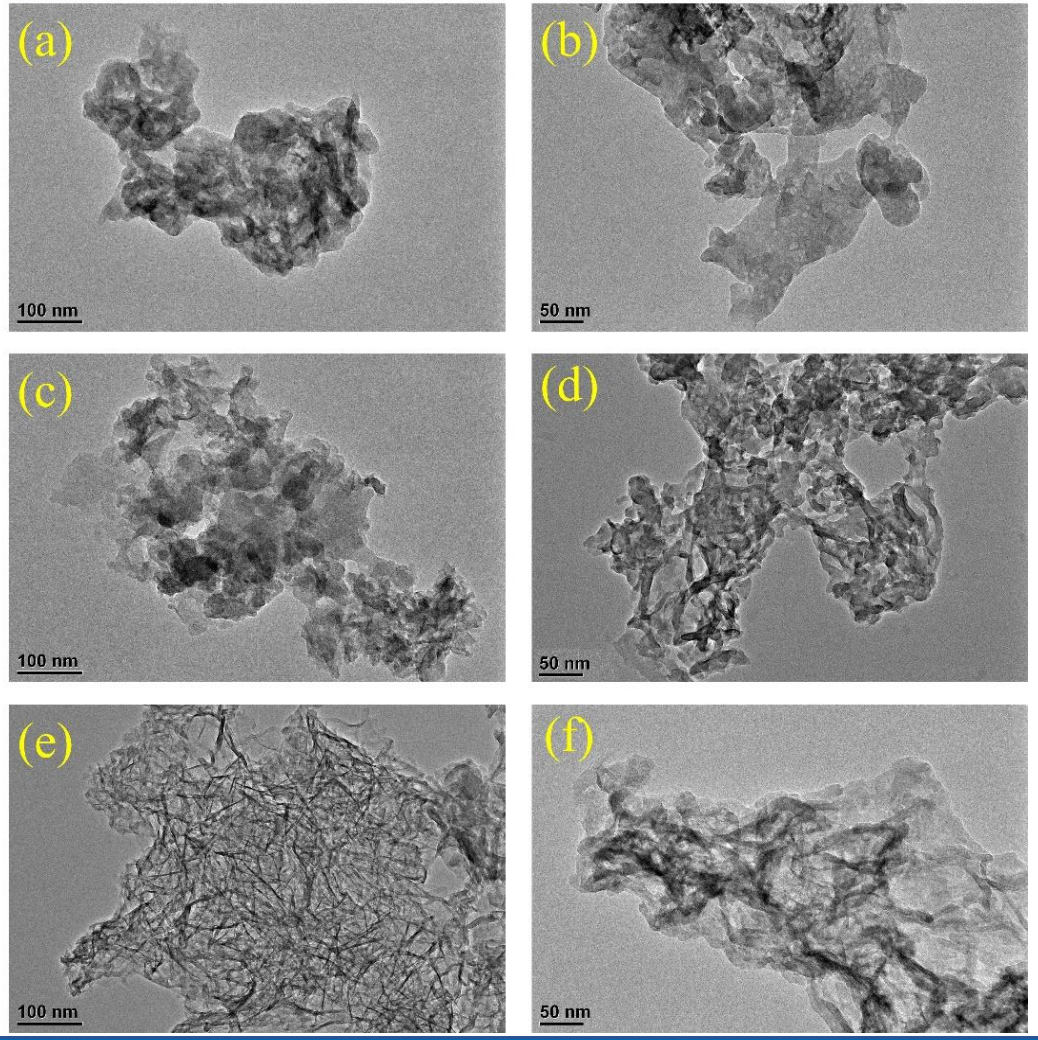
| Sample | C/S Ratio |
|---|---|
| Control | 1.0 |
| L-Asp-CSH | 0.9 |
| PDA-CSH | 0.9 |

# Characteristics of synthesized C-S-H

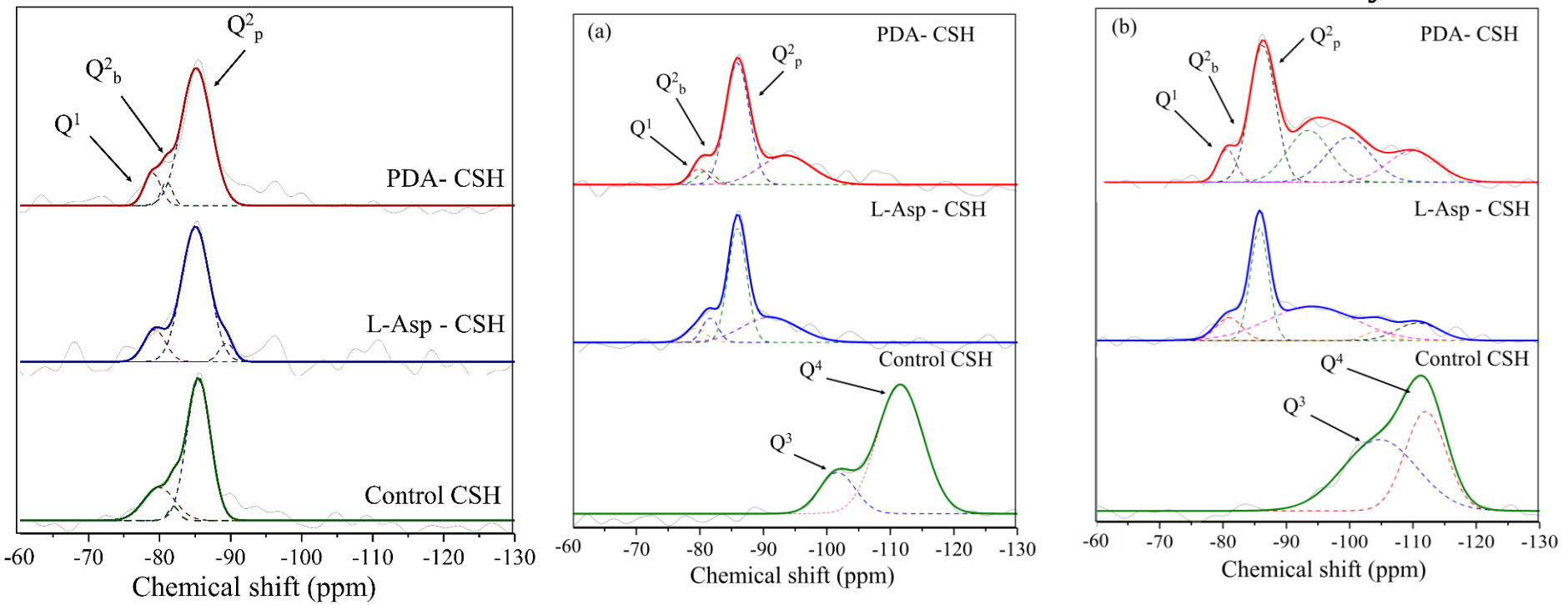
Control C-S-H

PDA modified C-S-H

L-Asp modified C-S-H

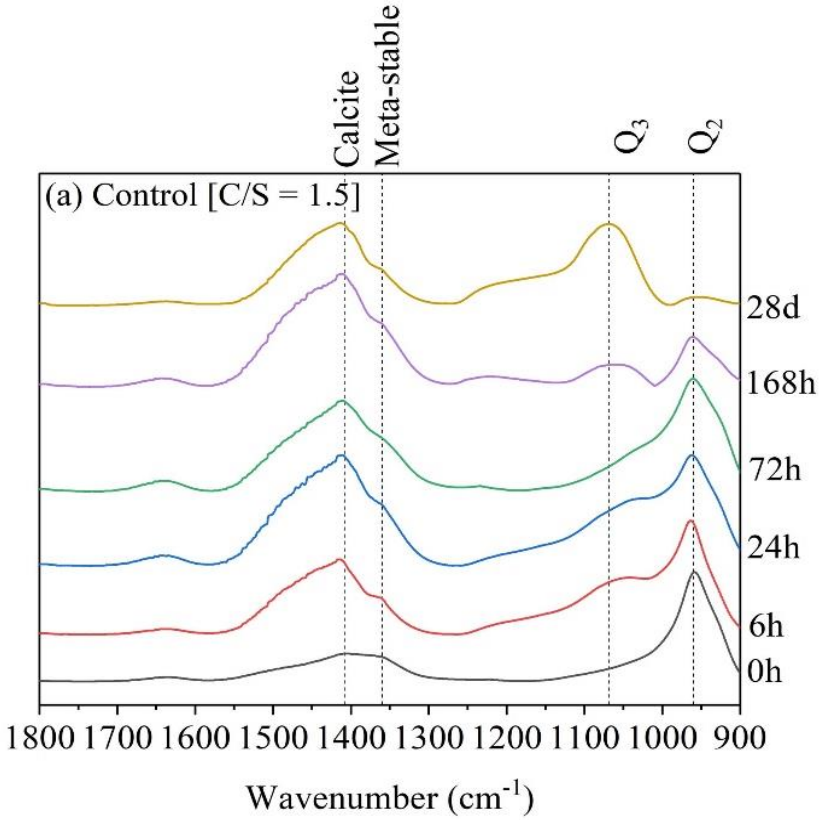


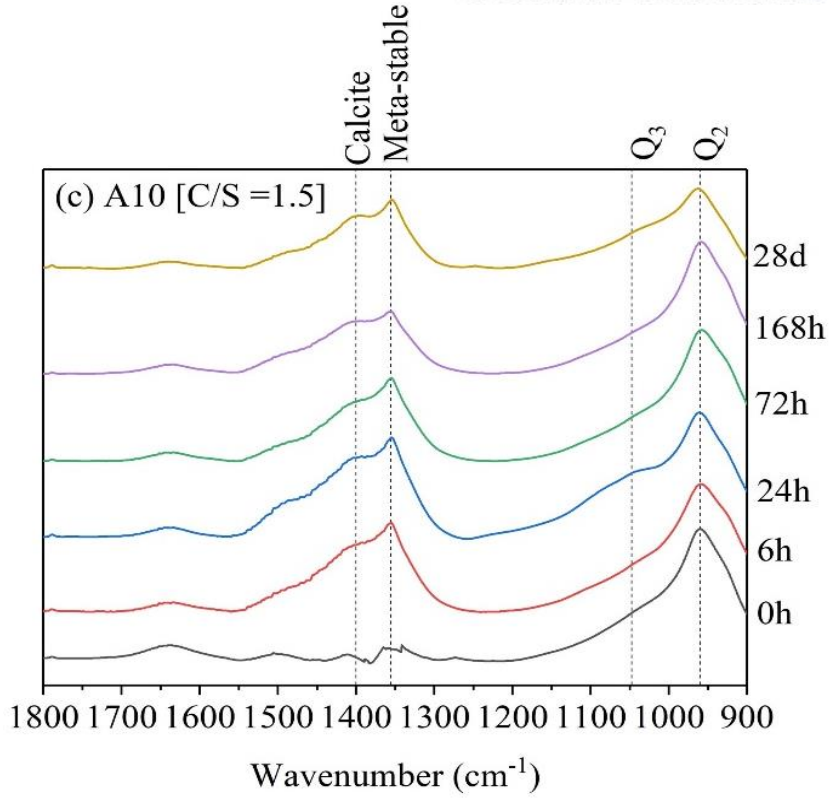
# Effects of Carbonation: $^{29}$Si NMR




**Both L-Asp and PDA modified batches showed superior resistance to carbonation**

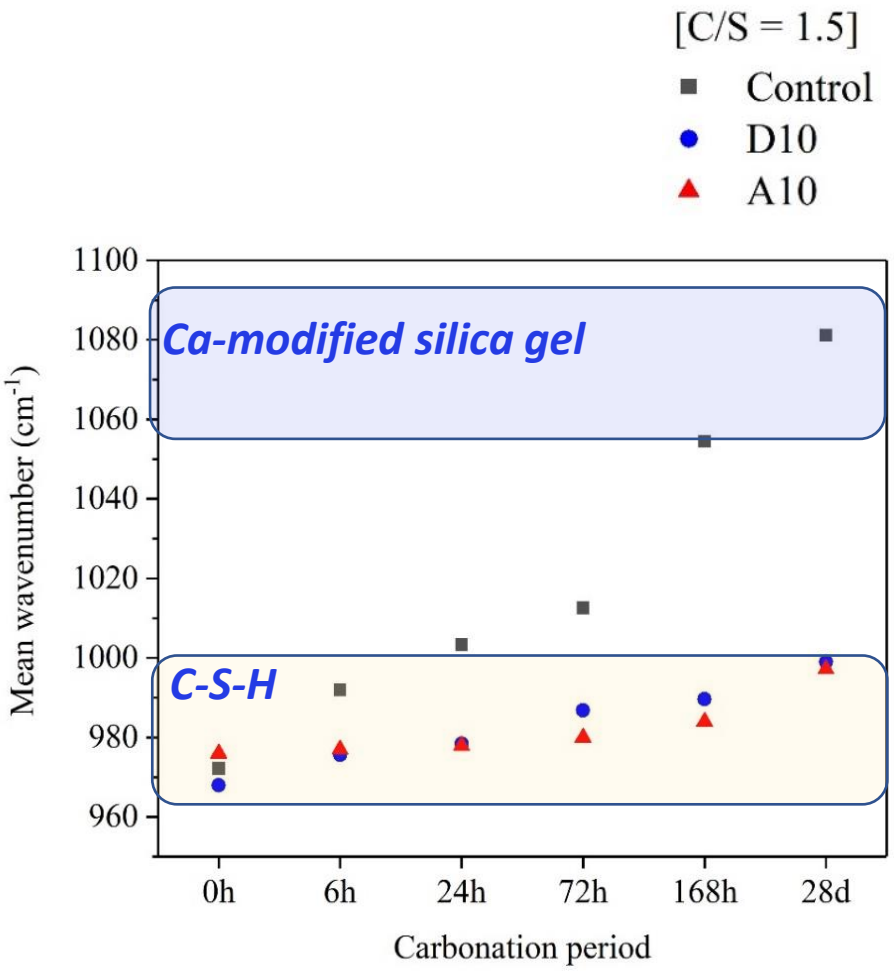
# Carbonate Polymorphs: FTIR spectra



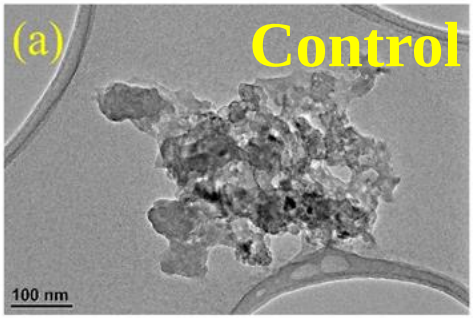



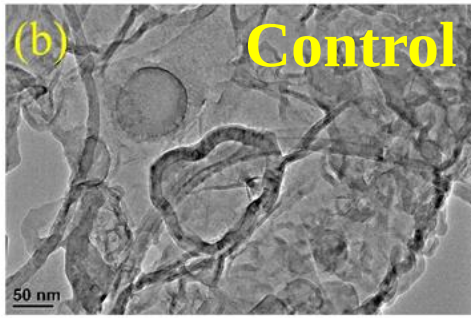

- Control batch primarily contained calcite
- L-Asp and PDA modified C-S-H primarily formed ACC and vaterite after carbonation

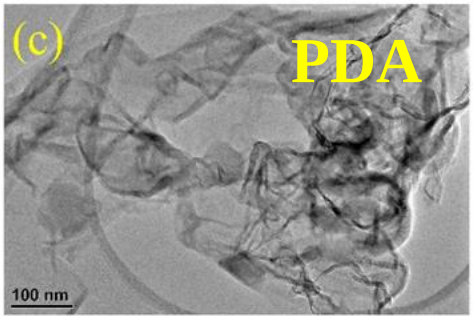
# Carbonation Degradation Rate

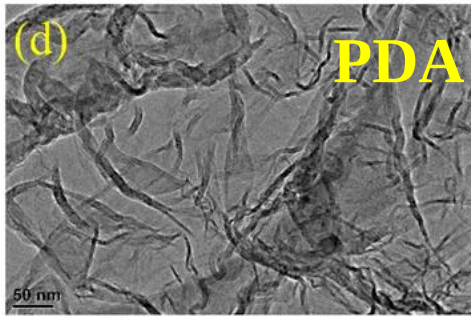


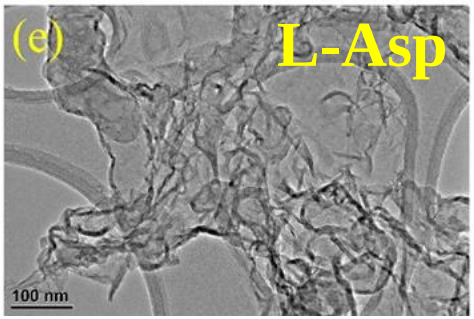

## After Carbonation

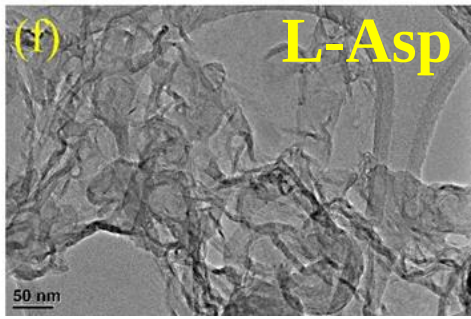


# Effects of Molecules and Carbonation:
## Nanomechanical properties

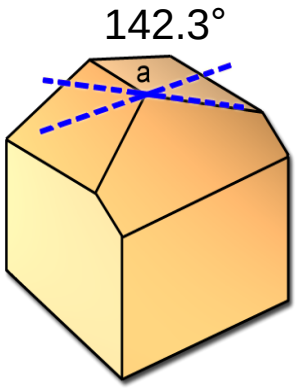



*Figure: Berkovich tip*

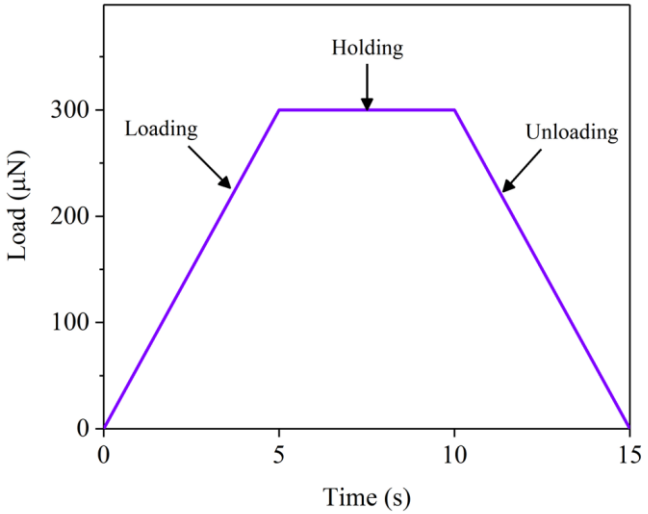



*Figure: Loading setup*

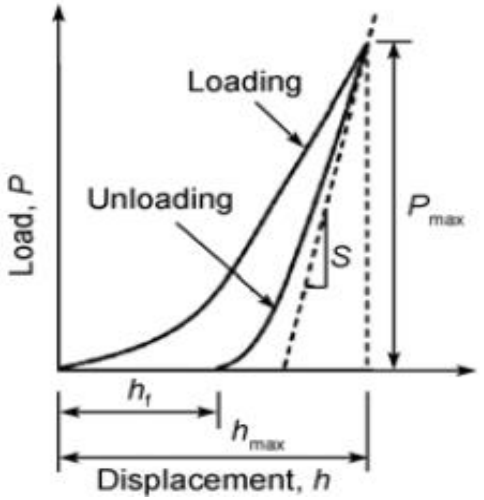
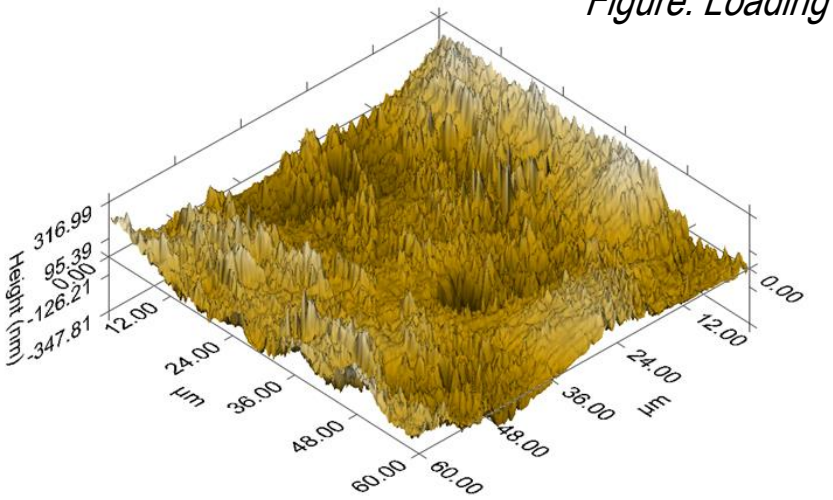


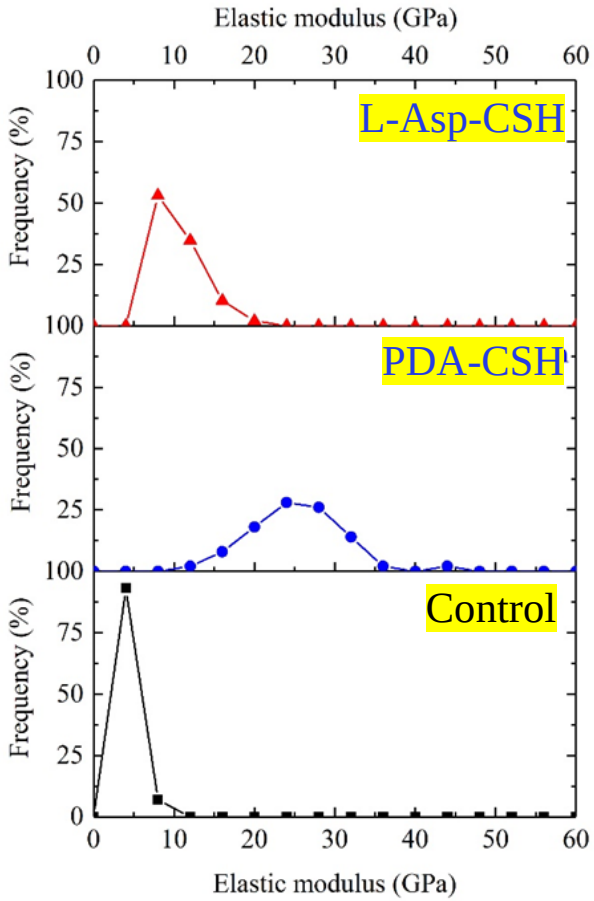

*Figure: Load vs. Displacement*



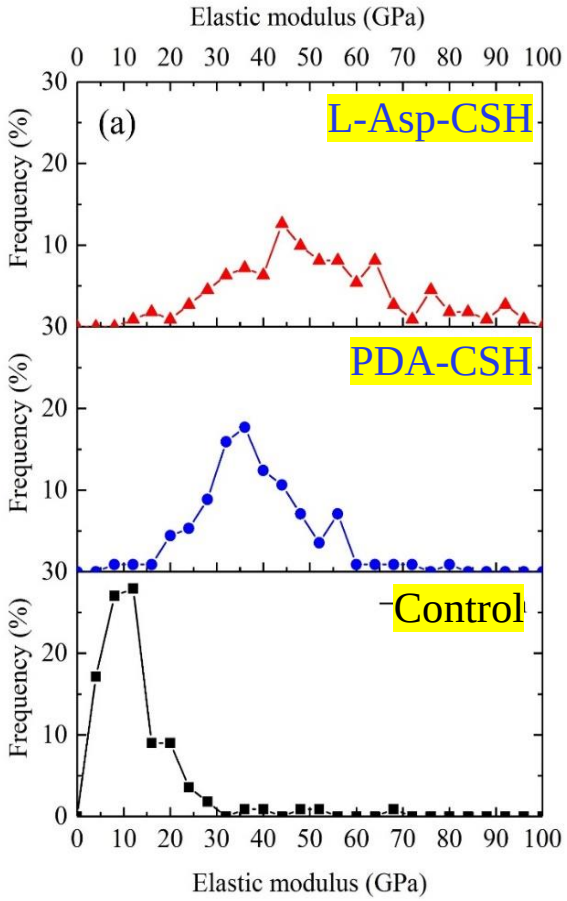

- **Grid nanoindentation**: 120 indentations performed
- **Scan size:** 30 μm x 30 μm (grid indentation performed twice over two area)
- **RMS roughness:** less than 80 nm
- **Peak load:** 300 μN force
- **Average indentation depth:** 100-300 nm

# Effects of Molecules and Carbonation:
## Nanomechanical properties

**Before Carbonation**



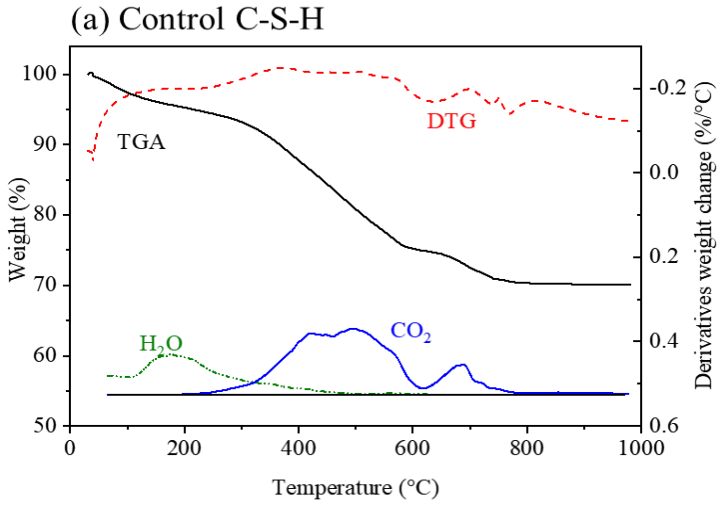

**After Carbonation (168 hours)**

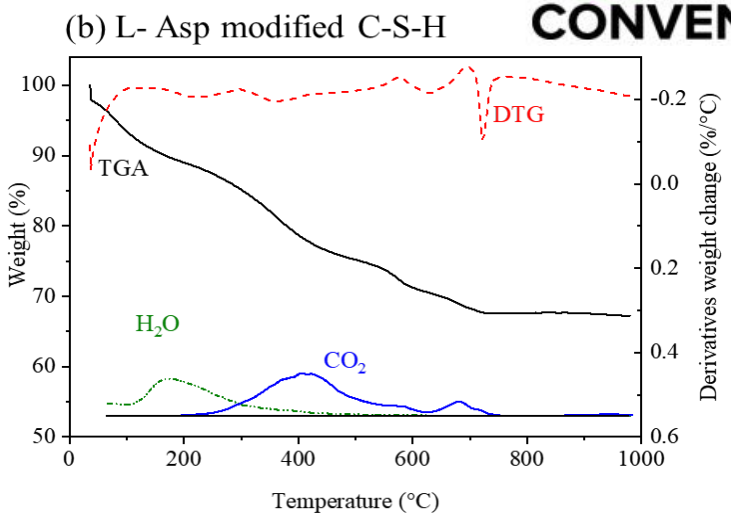


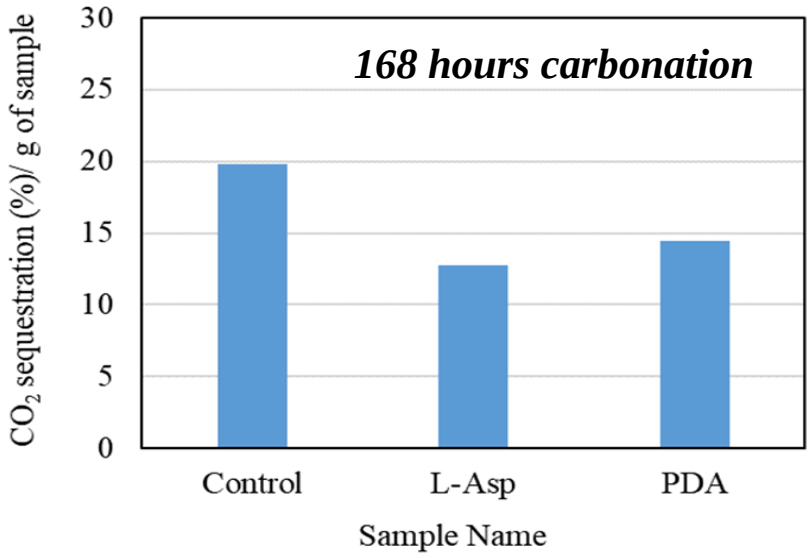

- Biomimetic molecules showed enhanced elastic modulus before and after carbonation

# Effects of Molecules:

## $CO_2$ sequestration capacity



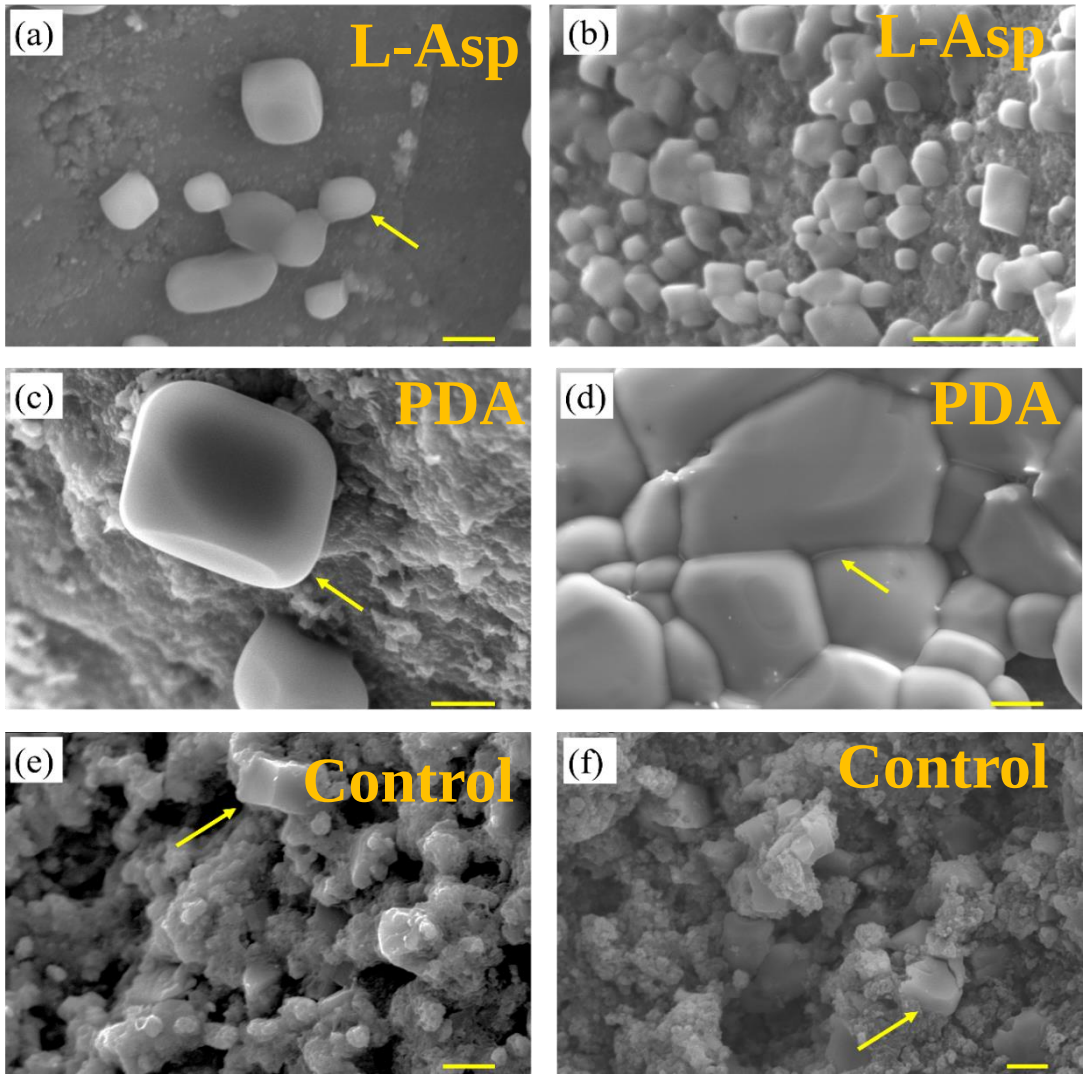




- Biomimetic molecules reduce $CO_2$ sequestration

# Effects of molecules:

## $CaCO_3$ morphology



# Concluding Remarks

- Biomimetic molecules can reduce or prevent carbonation degradation of C-S-H
- Biomimetic molecules can significantly enhance elastic properties of C-S-H
- These molecules can be used as chemical admixtures in some low-carbon binders, including alkali-activated materials, SCM containing concrete, etc.
- Selection/ screening of biomimetic molecules is challenging

## Acknowledgement


# Thank you!

Questions

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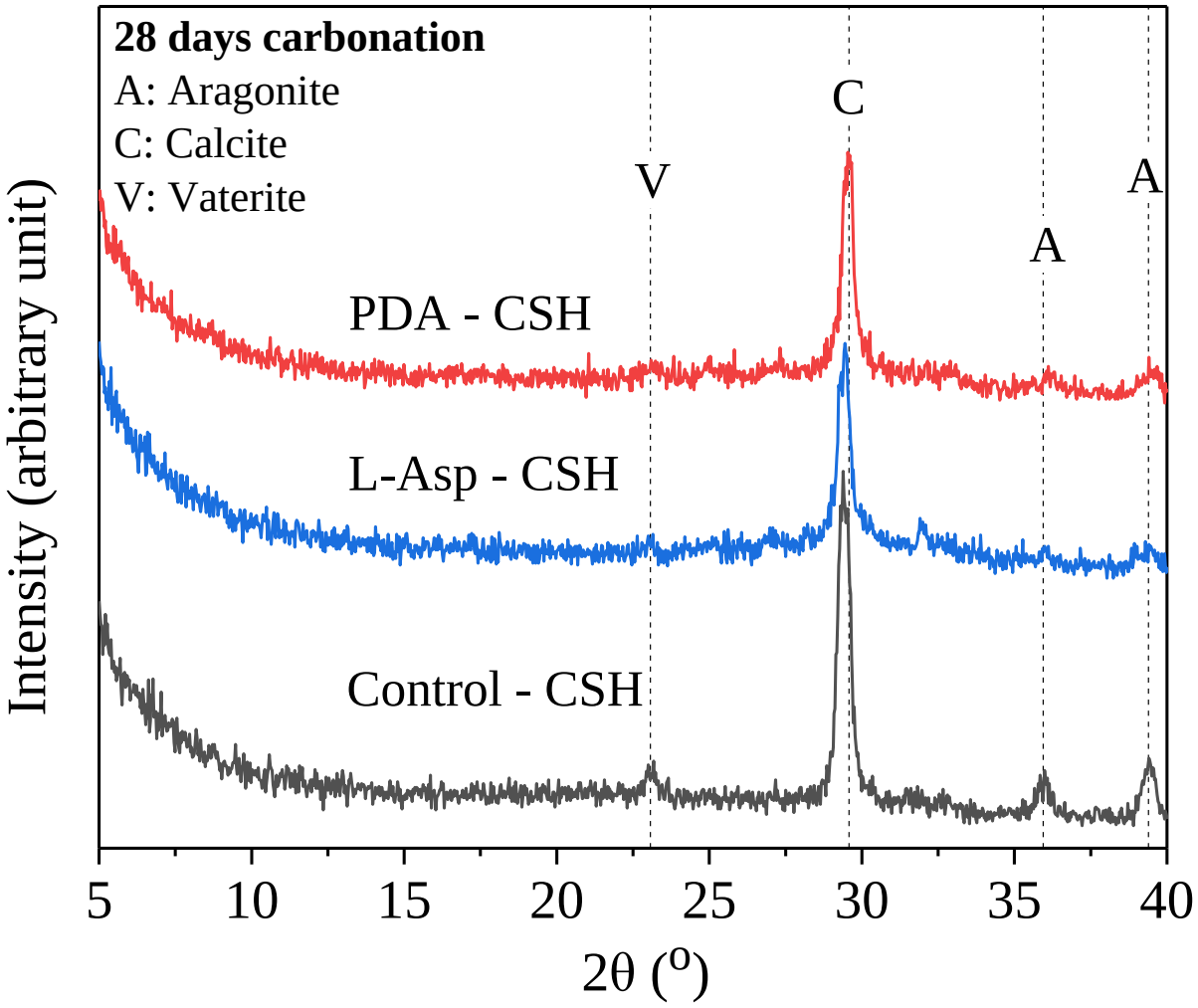
https://www.ashraf-lab.com/


28 days carbonation
A: Aragonite
C: Calcite
V: Vaterite
V
C
A
A
PDA - CSH
L-Asp - CSH
Control - CSH
Intensity (arbitrary unit)
5
10
15
20
25
30
35
40
2θ (º)