# CONCRETE AS A HIERARCHICAL STRUCTURAL COMPOSITE MATERIAL

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## MOTIVATIONS AND OBJECTIVES

•Production of cement contributes to up to 10% of world $CO_2$ emission.

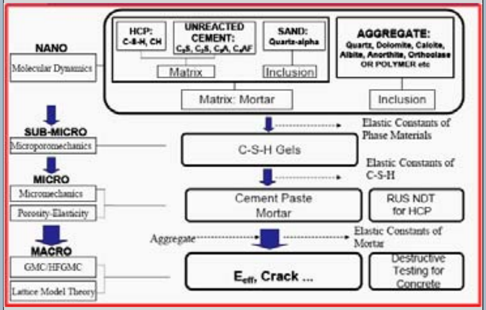
•Greener, more economical and more durable concrete.

•Nanoscale C-S-H still not fully understood

•Performing atomistic simulations to concrete constituent materials

•Setting a framework for understanding the relationship between the chemical composition, microstructure morphology and mechanical properties of concrete constituents

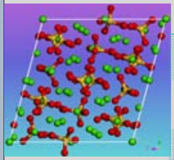
## A BIG PICTURE




## CEMENT

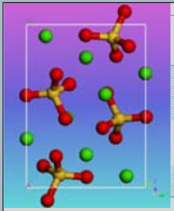
Molecular Dynamics Simulation

Commercial software Materials Studio was used



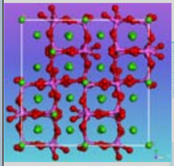
$C_3S$

| Supercell Properties | 1a×1b×1c | | | 2a×2b×2c | | | Ref Values |
|---|---|---|---|---|---|---|---|
| MD Tools & Forcefield | DC | FC | FU | DC | FC | FU | Nano-Inden |
| E | 168 | 137 | 45.4 | 139 | 148 | - | 135<br>117<br>60~300 |
| ν | 0.34 | 0.29 | 0.26 | 0.36 | 0.35 | - | 0.31 |



$C_2S$

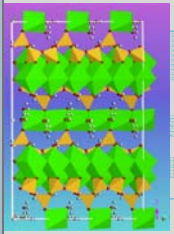
| Supercell Properties | 1a×1b×1c | | | 2a×2b×2c | | Ref Values |
|---|---|---|---|---|---|---|
| MD Tools & Forcefield | DC | FC | FU | DC | FC | Nano-Inden |
| E | 285 | 122 | 57.7 | 265 | 121 | 130 |
| ν | 0.2 | 0.19 | 0.35 | 0.22 | 0.19 | 0.31 |



$C_3A$

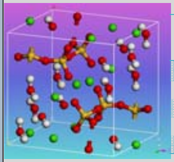
| Supercell Properties | 1a×1b×1c | | 2a×2b×2c | | Ref Values |
|---|---|---|---|---|---|
| MD Tools & Forcefield | FU | FD | FU | FD | Nano-Inden |
| E | 70 | 122 | 265 | 121 | 130 |
| ν | 0.31 | 0.19 | 0.22 | 0.19 | 0.31 |

## HYDRATED CEMENT



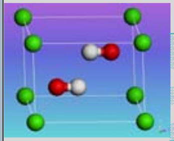
CSH: Tobermorite 14 Å

| Supercell Properties | 1a×1b×1c | | 2a×2b×2c | | Ref Results |
|---|---|---|---|---|---|
| | FU | DC | FU | DC | |
| E | 42.94 | 43.01 | 20.65 | **51.4** | 91 |
| ν | 0.29 | 0.343 | 0.4 | **0.328** | 0.17 |
| κ | 33.4 | 45.68 | 32.8 | **49.79** | 46 |
| G | 16.7 | 16.01 | 7.4 | **19.35** | 39 |



CSH: Jennite

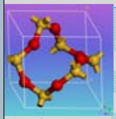
| Supercell Properties | 1a×1b×1c | | 2a×2b×2c | | Ref Results |
|---|---|---|---|---|---|
| MD Tools | FC | DC | FC | DC | |
| E | 44.1 | 82.2 | 66.9 | - | 66 |
| ν | 0.28 | 0.33 | 0.34 | - | 0.24 |
| κ | 33.3 | 78.4 | 69 | - | 43 |
| G | 17.2 | 31.0 | 25 | - | 26 |



CH

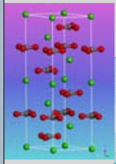
| Supercell Properties | 1a×1b×1c | | 3a×3b×3c | | 5a×5b×5c | | Ref Value |
|---|---|---|---|---|---|---|---|
| MD Tools & Forcefield | DC | FC | DC | FC | DC | FC | |
| E | 238.5 | **50.02** | 257.2 | 71.5 | 138.6 | - | 51.49 |
| ν | 0.321 | **0.31** | 0.243 | 0.28 | 0.36 | - | 0.23 |
| κ | 222.2 | **43.89** | 166.9 | 53.8 | 165.4 | - | 31.65 |
| G | 90.29 | **19.09** | 103.4 | 27.9 | 50.94 | - | 20.95 |

## SAND AND AGGREGATE



Quartz

| Supercell Properties | 1a×1b×1c | | 2a×2b×2c | | 3a×3b×3c | | 4a×4b×4c | Ref Value |
|---|---|---|---|---|---|---|---|---|
| MD Tools & Forcefield | DC | FC | DC | FC | DC | FC | DC | |
| E | 139.7 | 100 | **98.47** | 78 | 83.82 | 28 | 98.66 | 95.57 |
| ν | -0.208 | 0.34 | **0.106** | 0 | 0.106 | -0.2 | 0.109 | 0.08 |
| κ | 32.89 | 104 | **41.65** | 25.7 | 35.46 | 6.67 | 42.05 | 37.8 |
| G | 88.19 | 38 | **44.52** | 39.2 | 37.89 | 17.5 | 44.48 | 44.3 |

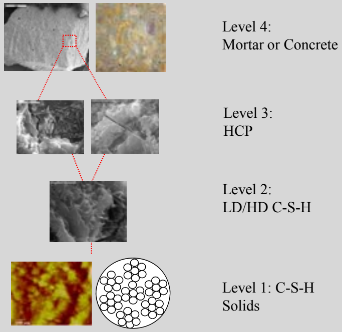


Calcite

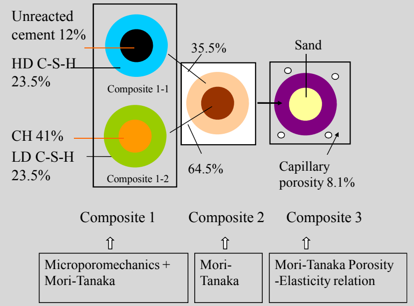
| Supercell Properties | 1a×1b×1c | | 2a×2b×2c | 3a×3b×3c | 4a×4b×4c | Ref Value |
|---|---|---|---|---|---|---|
| MD Tools & Forcefield | DC | FC | DC | DC | DC | |
| E | 159.5 | 193 | **97.83** | 103.5 | 96.38 | 95.57 |
| ν | 0.31 | 0.39 | **0.3** | 0.32 | 0.33 | 0.08 |

## CONCRETE AS A HIERARCHICAL COMPOSITE

Multi-Level Microstructure of Cement-Based Materials




A Proposed Cement Paste Model




Computation of Effective Properties of Concrete

Lattice Model

General Method of Cells

## RESULTS AND CONCLUSIONS

Experiment Validations

Resonant Ultrasound Spectroscopy Experiment to test Cement Paste

ASTM C469 for testing Young's Modulus and Poisson's Ratio

Results

| | Young's Modulus (GPa) |
|---|---|
| $E_{mortar}$ | 23.7 |
| $E_{mortar}$: RUS | 21.5 |
| $E_{con\_eff}$ : GMC | 42 |
| $E_{con\_eff}$ : Lattice | 36.3 |
| $E_{con\_eff}$ : Experiment | 38.2 |

Conclusions

•Molecular dynamics is a very useful tool in the computation of mechanical properties of cementitious materials.

•The hierarchical approach used in this study can be a powerful tool to investigate the properties of cement concrete from nanoscale to macroscale.

•A framework is set for the understanding of the relations among chemical composition, microstructure morphology, and the macroscale mechanical properties of concrete constituents

## ACKNOWLEDGEMENT

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