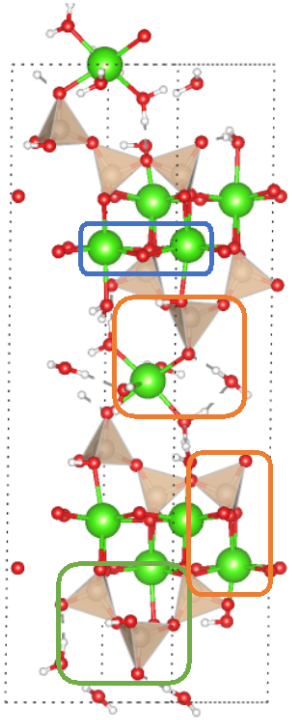
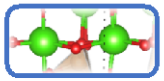
# Materials Research Science and Engineering Centers

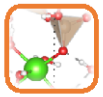
## Modeling the Early Stage Formation Mechanisms of Calcium Silicate Hydrates and Related Gels in Concrete (IRG-2)

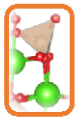
K. Yang[1] and C. E. **White**[1] arXiv:1903.10587v1 (2019). [1]Princeton University, USA



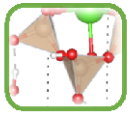


1 **$Ca(OH)(H_2O)^+$—$Ca(OH)(H_2O)^+$**





2 $Ca(H_2O)_6^{2+}$—$Si(OH)_3O(H_2O)^-$
$Ca(H_2O)_6^{2+}$—$Si(OH)_2O_2(H_2O)_5^{2-}$
**$Ca(OH)(H_2O)^+$—$Si(OH)_3O(H_2O)^-$**
**$Ca(OH)(H_2O)^+$—$Si(OH)_2O_2(H_2O)_5^{2-}$**



3 $Si(OH)_4$—$Si(OH)_4$
$Si(OH)_4$—$Si(OH)_3O(H_2O)^-$,
$Si(OH)_4$—$Si(OH)_2O_2(H_2O)_5^{2-}$
**$Si(OH)_3O(H_2O)^-$—$Si(OH)_3O(H_2O)^-$**

- Formation mechanism of calcium-silicate-hydrate gel (strength giving phase in concrete) is unknown
- Employed density functional theory to compute Gibbs free energies of reaction between various calcium and silicate species
- Proposed formation mechanism:
  1. Formation of calcium oxide layer
  2. Inclusion of silicates via interaction between calcium and silicate-bearing species
  3. Formation of silicate chains

Schematic representation of the bonding environments in calcium-silicate-hydrate gel (shown here as a tobermorite to aid visualization) and the early stage formation mechanisms involving select interactions between calcium- and silicon-bearing species identified by density functional theory calculations. Green: calcium atoms, brown: silicate tetrahedra, red: oxygen atoms, white: hydrogen atoms. Reactions in bold are considered more likely to happen for the given reaction type, and the numbering indicates the relative favorability of the reactions.

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