Supporting material

Hydration reactivity difference between dicalcium silicate and tricalcium silicate revealed from structural and Bader charge analysis

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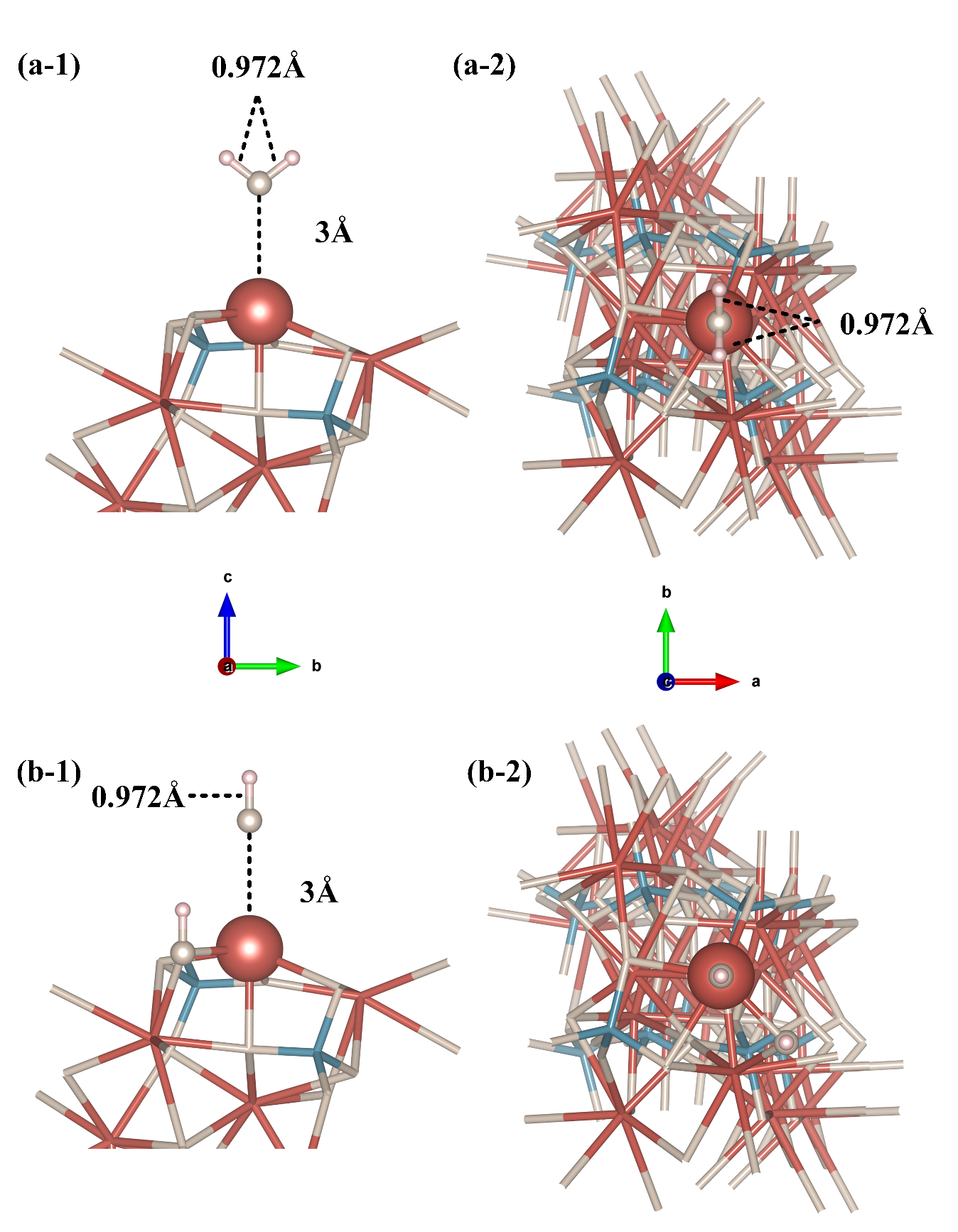
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**Table S1** Lattice parameters of β-C2S and M3-C3S (experimental measurements and DFT calculations)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Types | Volume(Å^3) | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) |
| β-C2S(Exp) | 343.91 | 5.50 | 6.75 | 9.30 | 90 | 94.59 | 90 |
| β-C2S(PBE) | 346.02 | 5.53 | 6.76 | 9.30 | 90 | 95.09 | 90 |
| β-C2S(PBEsol) | 334.02 | 5.46 | 6.68 | 9.20 | 90 | 95.26 | 90 |
| M3-C3S(Exp) | 722.32 | 9.30 | 7.08 | 12.22 | 90 | 116.08 | 90 |
| M3-C3S(PBE) | 717.60 | 9.28 | 7.11 | 12.16 | 90 | 116.56 | 90 |
| M3-C3S(PBEsol) | 689.55 | 9.12 | 7.05 | 11.98 | 90 | 116.38 | 90 |



**Fig. S1.** Initial structure of molecules and dissociative adsorption on the surface of β-C2S (001): **a-1)** Molecular adsorption, **a-2)** Molecular adsorption, **b-1)** Dissociative adsorption, **b-2)** Dissociative adsorption.