Supporting Information

Carbonation reaction mechanisms of portlandite predicted from enhanced ab-initio molecular dynamics simulations

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Convergence tests for the plane-wave cutoff energy

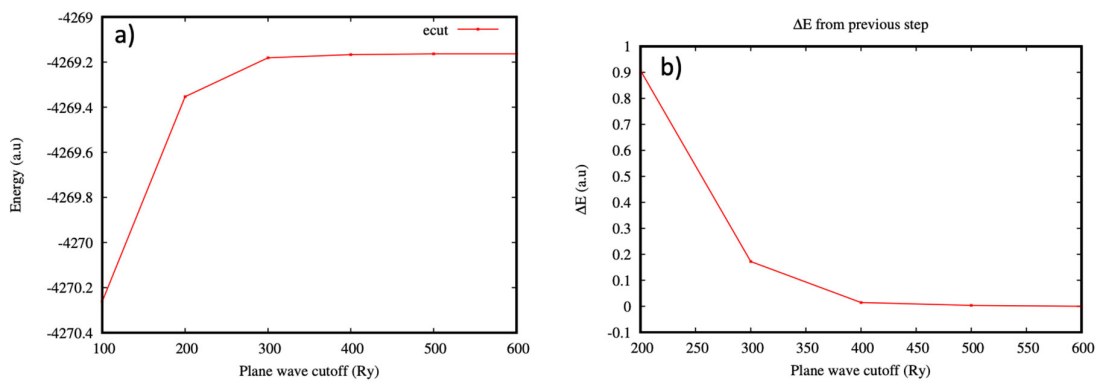

Figure S1: a) The variation of the total energy with the plane-wave basis cutoff energy. b) Energy change relative to the previous step. The value of 400 Ry is selected since there is negligible change in energy beyond this value.

Metadynamics simulations

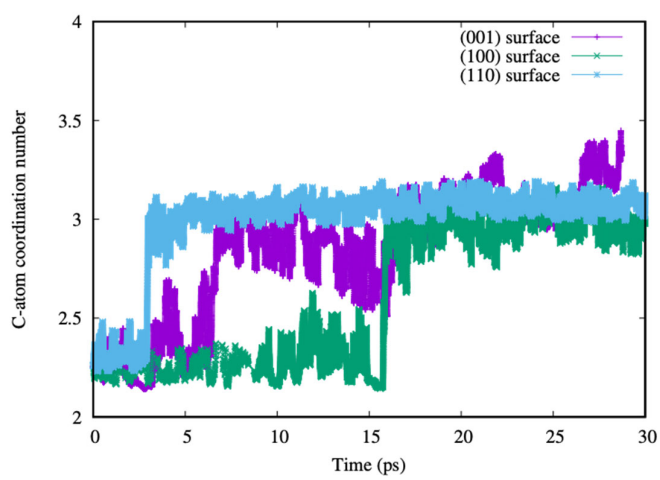

Figure S2: Variation of the Carbon atom coordination number (CV) with time for the metadynamics simulations of the portlandite/CO_2/H_2O systems.

Snapshots of the portlandite/CO_2/H_2O systems

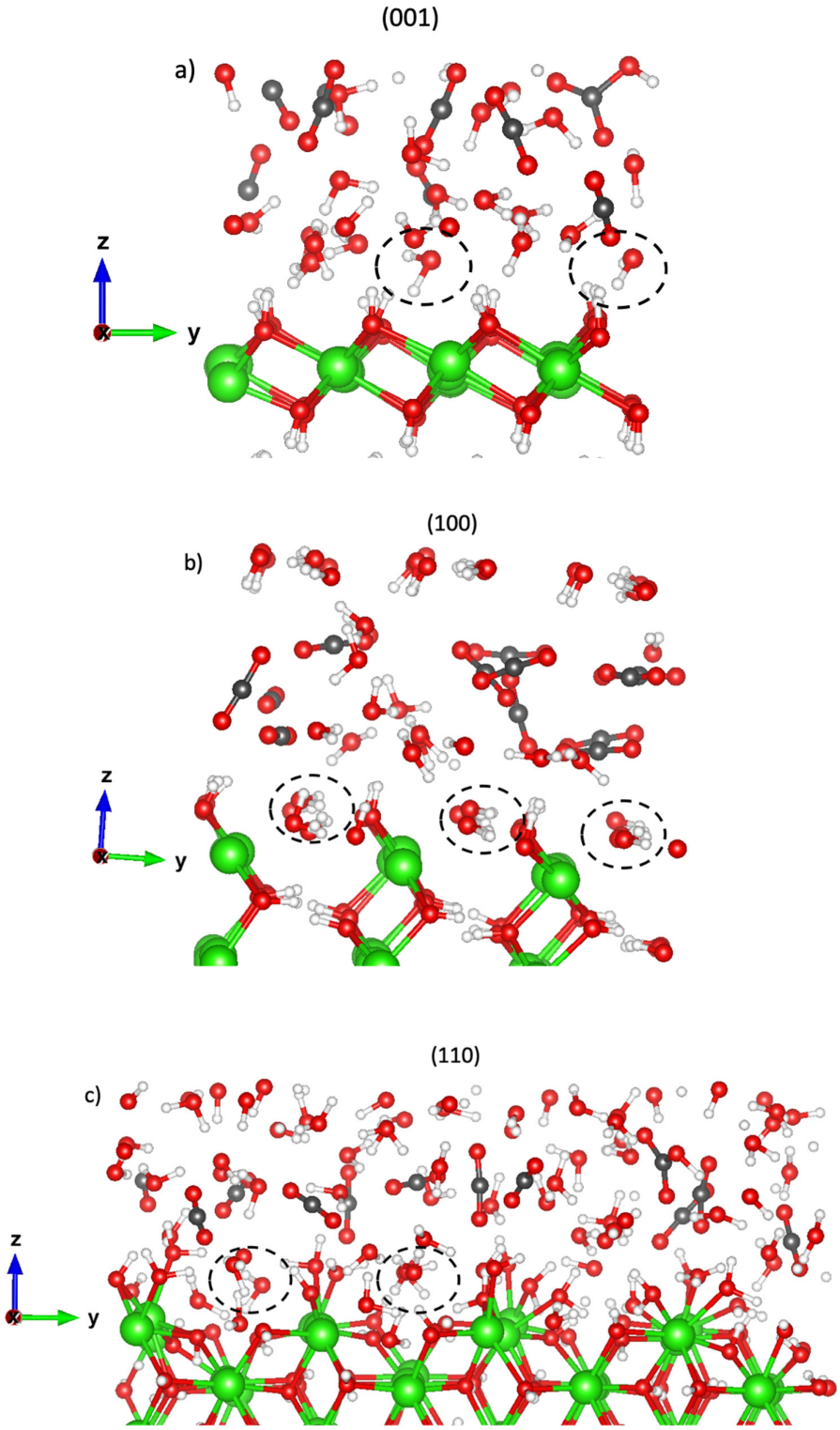

Figure S3: Snapshots of the a) (001), b) (100) and c) (110) portlandite pore systems with the positions of water molecules interacting with the surfaces highlighted by the dashed circles.