

Supplementary Information For

First Principles Simulations of MgO (100) Surface Hydration at Ambient Conditions

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CONTENT

Figure S1: Bulk structure of Mg(OH)₂

S2

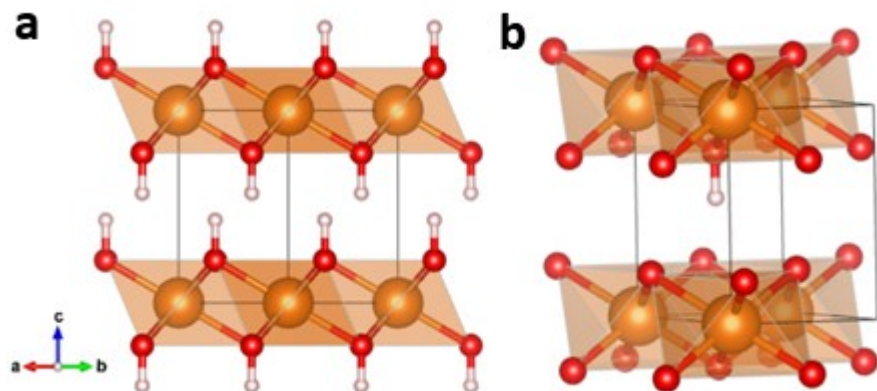


Figure S1: (a) Structure of bulk Mg(OH)₂ and (b) representation of the local environment of a OH group. Some atoms have been removed for clarity.