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Supporting Information for

Alkaline Earth Metal Oxide Nanocluster Modification of Rutile TiO₂ (110) promotes Water Activation and CO₂ Chemisorption

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This supporting information document contains the following material

Table S1: Effect of plane wave cut off energy on selected adsorption energies

Figure S1: Transition state for water dissociation on (MgO)₄-rutile

Figure S2: Spin density plot for the triplet electronic state in CO_2 adsorbed on $(MgO)_{4^-}$, $(CaO)_{4^-}$ and $(BaO)_{4^-}$ rutile

Cut off Energy / eV	E ^{ads} (H ₂ O)	E ^{ads} (CO ₂)
(MgO) ₄ -rutile		
396	-1.28 (molecular)	-0.63 (linear)
	-3.27 (dissociated)	-2.24 (carbonate)
500	-1.26 (molecular)	-0.59 (linear)
	-3.32 (dissociated)	-2.18 (carbonate)
(CaO) ₄ -rutile		
396	-3.69	-3.99
500	-3.70	-3.94
(BaO) ₄ -rutile		
396	-2.57	-3.36
500	-2.57	-3.39

Table 1: Effect of cut-off energy on adsorption energies of water and CO_2 at alkaline earth oxide modified rutile TiO_2 .



Figure S1: Transition state for water dissociation on (MgO)₄-rutile (110).



Figure S2: Atomic structure and spin density isosurfaces for the triplet electronic state for CO_2 adsorbed at **(a):** $(MgO)_4$ -rutile, **(b):** $(CaO)_4$ -rutile and **(c):** $(BaO)_4$ -rutile where CO_2 is adsorbed as a carbonate