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Supplementary Information: Modelling silicate mineral interfaces for carbon dioxide sequestration: structure and stability of orthoenstatite surfaces.†

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1 Force field parameters

Charges in $|e|$ are: +2.00 (Mg), +2.10 (Si), -1.45 (O_1 bound to only one Si), -1.2 (O_2 bound to two Si, linking SiO_4 tetrahedra).

A Buckingham potential has been used to describe all interactions with oxygen atoms, with a cutoff of 9 Å:

$$E = A\ exp\Big(-\frac{r}{\rho}\Big) - \frac{C}{r^6} \quad (1)$$

C has been set to 0 for all interactions, whereas A and ρ parameters for each couple of atoms are reported in Table 1.

Table 1 A [eV] and ρ [Å] parameters used in Equation 1.

atom	atom	A	ρ
O_1	O_1	54874.441	0.216923
O_1	O_2	4116.0017	0.286567
O_2	O_2	24125772.	0.140258
O_1	Si	260475.50	0.125449
O_2	Si	328096.04	0.122843
O_1	Mg	89566.207	0.168164
O_2	Mg	43025618.	0.116092

2 Additional surfaces

Graphical representation of $\{hk0\}$ surfaces with $d_{hkl} > 2.5$Åthat are not documented in the literature is reported in Figure 1. As discussed in the paper, these are all microfacets. Their lattice parameters, d_{hkl} and surface energy as calculated with the force field are reported in the main text.

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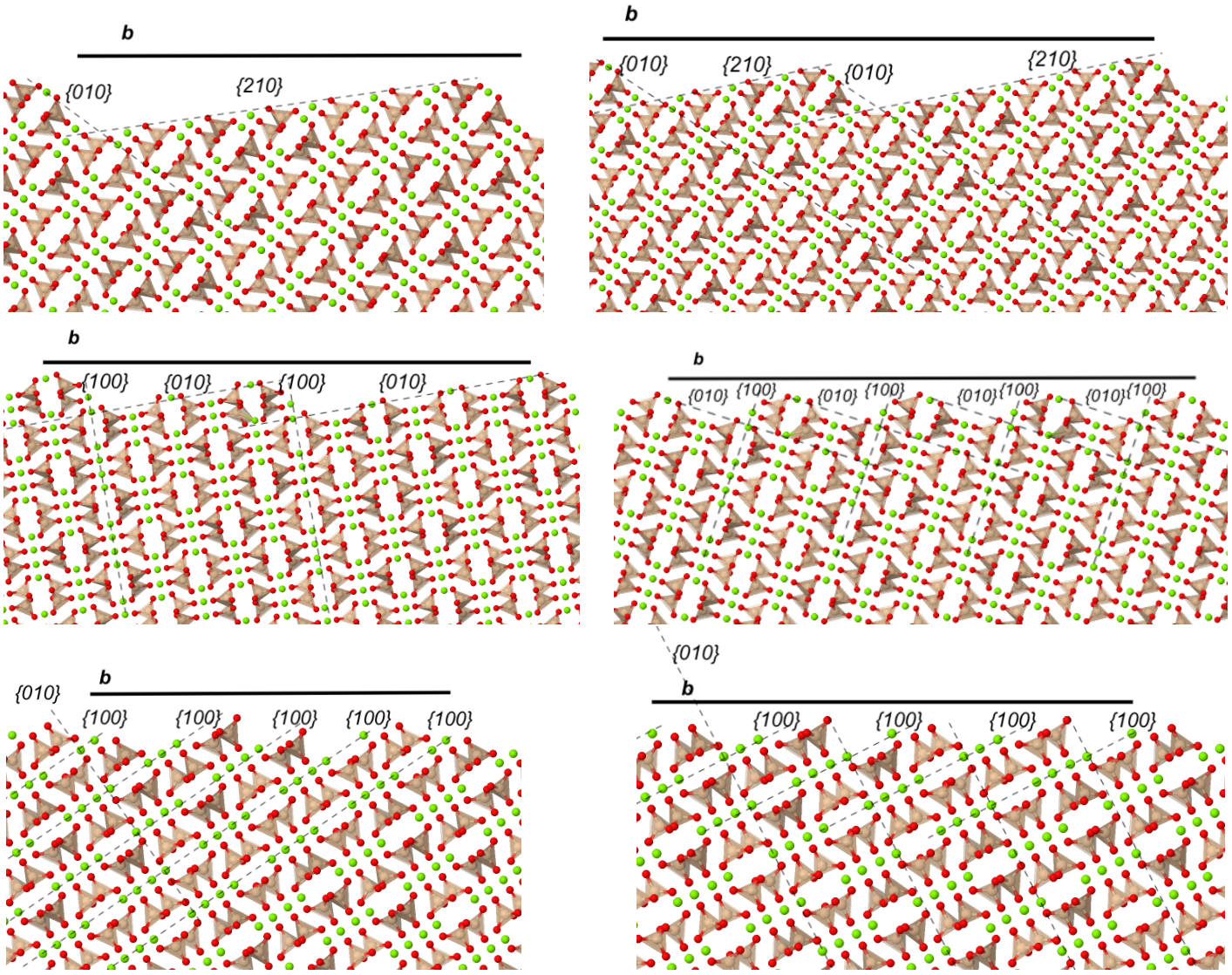

Fig. 1 View along x of $\{320\}$ (top left), $\{430\}$ (top right), $\{130\}$ (centre left), $\{230\}$ (centre right), $\{310\}$ (bottom left), $\{410\}$ (bottom right) surfaces as obtained from cutting the bulk. The b lattice parameter is shown as a measure of the size of the unit cell; the microfacets are highlighted with a dotted line and their orientation is reported. SiO_4 tetrahedra are coloured in brown, oxygen atoms in red and magnesium atoms in green.