NC-AFM studies of the $CaSiO_3$ (100) surface with adsorbed CO_2 and H_2O

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The interaction of wollastonite ($CaSiO_3$), a silicate mineral, with CO_2 and water is highly relevant in the field of carbon capture [1], rock weathering [2] and cement production [3]. We have investigated the preferentially cleaved (100) surface in ultrahigh vacuum (UHV) and exposed it to controlled amounts of H_2O and CO_2 at 100 K. Using non-contact atomic force microscopy (NC-AFM) with functionalised tips, combined with ab-initio density functional theory (DFT) and AFM-simulations [4], we determined the atomic structure of the cleaved surfaces and the adsorption configurations of H_2O and CO_2. The cleaved surface exposes rows of alternating calcium and oxygen atoms. Between these rows, water adsorbs molecularly and without a barrier in a nested position, which was not reported in previous literature. The nested H_2O molecule aids the adsorption of the CO_2, which in turn forms a carbonate-like structure due to its interaction with the surface. At higher coverage, the strongly bound water forms regular patterns.

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[2] D. Feng, et al. J. Clean. Prod., **414**, 137625 (2023).
[3] H. Huang, et al. J. Clean. Prod., **211**, 830 (2019).
[4] N. Oinonen, et al. Comput. Phys. Commun., **305**, 109341 (2024).

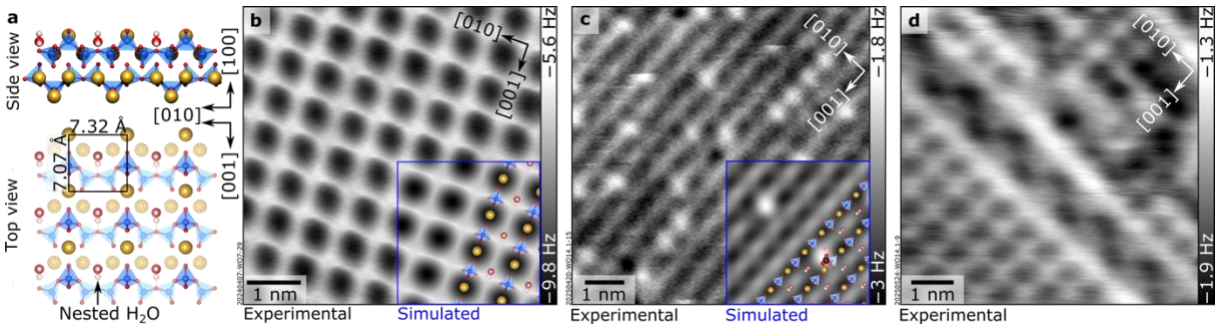

Figure 1. Wollastonite (100) surface: (a) DFT-optimised structure with one 'nested' H_2O per unit cell. (b) 5.5 x 5.5 nm² nc-AFM image of the cleaved surface reacted with H_2O at room temperature, overlaid with the DFT-derived AFM simulation. (c) 9.0 x 9.0 nm² nc-AFM image of the surface with adsorbed CO_2, overlaid with the simulation. (d) 7.0 x 7.0 nm² nc-AFM image showing the second and partial third layer of adsorbed H_2O molecules.