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Synergistic adsorptions of Na_2CO_3 and Na_2SiO_3 on calcium minerals revealed by spectroscopic and *ab initio* molecular dynamics studies

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The synergistic effects between sodium silicate (Na_2SiO_3) and sodium carbonate (Na_2CO_3) adsorbed on mineral surfaces are not yet understood, making impossible to finely tune their respective amount in various industrial processes. In order to unravel this phenomenon, diffuse reflectance infrared Fourier transform and X-ray photoelectron spectroscopies were combined with *ab initio* molecular dynamics to investigate the adsorption of Na_2SiO_3 onto bare and carbonated fluorite (CaF_2), an archetypal calcium mineral.

Both experimental and theoretical results proved that Na_2CO_3 adsorbs onto CaF_2 with a high affinity and forms a layer of Na_2CO_3 on the surface. Besides, at low Na_2SiO_3 concentration, silica mainly physisorbs under a monomeric protonated form, $Si(OH)_4$, while at larger concentration, significant amounts of polymerized and deprotonated forms are identified. A prior surface carbonation induces an acid-base reaction on the surface, which results in the formation of $SiO(OH)_3^-$ and $Si_2O_3(OH)_4^{2-}$, even at low coverage. Their adsorption is highly favoured compared to the acid forms, which explains the synergistic effects observed when Na_2SiO_3 is used after Na_2CO_3. Hence, when Na_2CO_3 is used during a separation process, lower Na_2SiO_3 concentrations are needed to obtain the same effect as with lone Na_2SiO_3 [Y. Foucaud, M. Badawi et al. *Chem. Sci.* 10 (2019) 9928].