Synergistic adsorptions of Na$_2$CO$_3$ and Na$_2$SiO$_3$ on calcium minerals revealed by spectroscopic and \textit{ab initio} molecular dynamics studies

M. BADAWI*, Y. FOUCAUD, L. FILIPPOV, O. BARRES, I. FILIPPOVA, S. LEBÉGUE
Université de Lorraine & CNRS, Nancy, France.
*michael.badawi@univ-lorraine.fr

The synergistic effects between sodium silicate (Na$_2$SiO$_3$) and sodium carbonate (Na$_2$CO$_3$) 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 \textit{ab initio} molecular dynamics to investigate the adsorption of Na$_2$SiO$_3$ onto bare and carbonated fluorite (CaF$_2$), an archetypal calcium mineral. Both experimental and theoretical results proved that Na$_2$CO$_3$ adsorbs onto CaF$_2$ with a high affinity and forms a layer of Na$_2$CO$_3$ on the surface. Besides, at low Na$_2$SiO$_3$ 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$_2$O$_3$(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$_2$SiO$_3$ is used after Na$_2$CO$_3$. Hence, when Na$_2$CO$_3$ is used during a separation process, lower Na$_2$SiO$_3$ concentrations are needed to obtain the same effect as with lone Na$_2$SiO$_3$ [Y. Foucaud, M. Badawi et al. \textit{Chem. Sci.} 10 (2019) 9928].