Atomistic simulations of organic inhibitors films in concrete

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Abstract
Corrosion inhibitors are largely used to prevent chloride-induced corrosion in reinforced concrete structures. The interaction mechanisms with the passive film present on steel still requires deeper understanding. Theoretical studies based on Molecular Mechanics and Molecular Dynamics can be useful in order to understand the strength of interaction and possible passivated thick film formations. In a previous work [1] based on molecular mechanics and molecular dynamics methods [2-5] organic inhibitors adsorbed on γ-FeOOH, comparing theoretical results with experimental data [1], were considered. The initial interaction with the inhibitor film and chlorides was studied. In particular, the adsorbed tartrate monolayer show the best behavior thanks to the repulsions by the COO^- groups exposed to chlorides, more distant from the γ-FeOOH surface, whereas the dimethylethanolamine film doesn't display the same repulsion. The molecular simulations are a useful tool to better understand the behaviour of inhibitors in presence of chlorides in order to better study the kinetics of the adsorption on passivated film, the first step of the corrosion that can take place and that it is important to prevent.

References
M.V. Diamanti, E. A. Pérez-Rosales, G. Raffaini, F. Ganazzoli, A. Brenna, M. Pedeferri, M. Ormellese, *Corrosion Science*, 100, 231-241 (2015).
G. Raffaini, F. Ganazzoli, *J. of Applied Biomat. & Biomachanics*, 8, 135-145 (2010).
G. Raffaini, S. Elli, F. Ganazzoli, *J. of Biomed. Mat. Res*. PART A, 3, 77A (2006).
G. Raffaini, L. Melone, C. Punta, *Chem. Comm*., 49, 6567-7670 (2013).
G. Raffaini, F. Ganazzoli, *J. of Biomed. Mat. Res*. PART A, 92A, 1382-1391 (2006).