

Understanding surface interactions in aqueous miscible organic solvent treated layered double hydroxides

VALENTINA ERASTOVA¹, MATTEO DEGIACOMI²,
DERMOT O'HARE², CHRIS GREENWELL³

¹ Department of Earth Sciences, Durham University, South Road, Durham DH1 3LE, U.K.

valentina.erastova@durham.ac.uk

² Chemistry Research Laboratory, Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA, U.K.

³ Department of Earth Sciences, Durham University, South Road, Durham DH1 3LE, U.K.

Layered materials are of interest for use in a wealth of technological applications, many of which require a high surface area for optimal properties and performance. Recently, an industrially scalable method to create high surface area layered double hydroxide (LDH) materials, which may be readily dispersed in non-polar solvents, has been developed[1]. This method involves treatment of LDHs with aqueous miscible organic (AMO) solvents. Here, molecular modeling is exploited to elucidate the AMO solvent-LDH interactions to understand how the dispersion process is facilitated by the AMO treatment. The simulations show mechanism of hydrogen-bond network disruption within the LDH interlayer by AMO solvents, leading to delamination[2].

[1] Yang M, McDermott O, Buffet JC, O'Hare D. Synthesis and characterisation of layered double hydroxide dispersions in organic solvents. RSC Advances. 2014

[2] Erastova V, Degiacomi MT, OHare D, Greenwell C. Understanding Surface Interactions in Aqueous Miscible Organic Solvent Treated Layered Double Hydroxides. RSC Advances. 2016