

Horizontal and vertical orders of water at mineral interfaces: a new paradigm for the BIL structural organization

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We will present some of our most recent theoretical DFT-MD and FF-MD simulations on aqueous mineral interfaces that will show how the balance between the vertical and horizontal structural order of the water in the Binding Interfacial Layer (BIL) at solid interfaces triggers the final structure of BIL-water. We will associate SFG (Sum Frequency Generation) and THz-IR spectroscopic signatures to these structural orders, combining theoretical and experimental spectroscopic data and structural assignments. The combination of SFG and THz-IR spectroscopies will be shown a compelling tool to characterize the finest details of molecular hydrophobicity/hydrophilicity at aqueous interfaces. This opens perspectives in the rationalization and optimization of local hydrophobic/hydrophilic effects, and in the design of aqueous interfaces.

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Some recent publications on these topics: [1] S. Pezzotti, A. Serva, F. Sebastiani, F. Siro Brigiano, D.R. Galimberti, L. Potier, S. Alfarano, G. Schwaab, M. Havenith, M.-P. Gageot, J. Phys. Chem. Letters, 12:3827 (2021) [2] J.D. Cyran, M.A. Donovan, D. Vollmer, F. Siro-Brigiano, S. Pezzotti, D.R. Galimberti, M.-P. Gageot, M. Bonn, E.H.G. Backus, PNAS 116 :1520-25 (2019) [3] F. Creazzo, D.R. Galimberti, S. Pezzotti, M.-P. Gageot J. Chem. Phys. 150:041721-18 (2019) [4] S. Pezzotti, D. Galimberti, , Y.R. Shen, M.-P. Gageot Phys. Chem. Chem. Phys., 20:5190-5199 (2018) [5] S. Pezzotti, D. R. Galimberti, M.-P. Gageot, Phys. Chem. Chem. Phys. 21:22188-22202 (2019)