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Water Adsorption on the Gypsum (010) Surface: a theoretical and experimental study[1] LUANA PEDROZA, FABIO RIBEIRO, GUSTAVO DALPIAN, Universidade Federal do ABC - Brazil, JACIARA DE CARVALHO SANTOS, PAULO B. MIRANDA, Instituto de Fsica de So Carlos, Universidade de So Paulo, Brazil — In this work we present a combined experimental/theoretical study which provides a molecular-level understanding of the ubiquitous and important gypsum/water interface. We investigate the structural and dynamic properties of adsorbed water on (010) gypsum single crystal surface, at room temperature, combining Sum Frequency Generation (SFG) Spectroscopy experiments and first principles simulations. Gypsum is a layered crystal with molecular planes linked through weak hydrogen bonding, allowing the perfect cleavage of (010) faces. The SFG spectra of gypsum in low relative humidity (RH) 0.1% under N_2 atmosphere showed anisotropic arrangement of H_2O structural molecules and the presence of dangling OH groups. When studying higher RH the adsorbed water also revealed an anisotropic arrangement although different than the one present in the structural water and with the free OH signal significantly suppressed. The theoretical results corroborates the experimental ones and allows to identify the structure of the water molecules at the interface.

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