

Structure and hydration of the FeS mackinawite/water interface from molecular modelling

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FeS mackinawite, the first condensed iron-sulphide phase in water, has a key role in the “iron-sulfur world” theory [1]. FeS has been postulated to be the catalytic driving force behind the formation of the first simple organic molecules in deep ocean hydrothermal vents. Thus, in order to properly account for the effects of the aqueous environment in the prebiotic reactions, it is crucial to achieve a detailed understanding of the mineral/solvent interactions. Despite its geochemical importance, and in contrast to the most common FeS₂ pyrite/water system [2] [3], our knowledge of the FeS/water interface remains limited [4].

Computer simulations can provide important insights into the chemical and physical properties of interfacial water. In this work, we employ classical molecular dynamics simulations to unravel the interplay between the most stable (001) mackinawite termination and water (Figure 1). We report the adsorption structures and energies at different solvent coverages, together with the water density profiles with respect to the distance from the surface. We compare the scenarios emerging both from ambient and extreme aqueous conditions, the latter typical of hydrothermal vents. Finally, we discuss the significant changes at the interface induced by the consideration of a more realistic defective substrate.

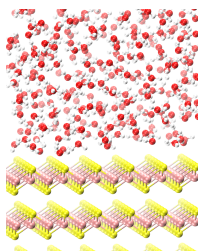


Figure 1:
FeS/water interface

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[3] Guevremont J. M. *et al.*, (1998) *Langmuir*, **14**, 1361-1366.
[4] Wittekindt C. *et al.*, (2012) *J. Chem. Phys.*, **137**, 054710.