

Abstract Submitted  
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**Dissociation of water and Acetic acid on PbS from first principles<sup>1</sup>**

ALESSANDRA SATTA, PAOLO RUGGERONE, CNR-INFM SLACS, GIOVANNI DE GIUDICI, Dept. Earth Science, University of Cagliari — The adsorption of complex molecules at mineral surfaces are crucial ingredients for understanding the mechanisms that rule the interaction between minerals and the biosphere and for predicting both the stability and the reactivity of minerals. The present work focuses mainly on the early stages of different adsorption reactions occurring at both the cleavage surface and a high-index vicinal surface of galena (PbS). We have studied the dissociation mechanism of water and acetic acid on the galena surfaces by means of ab initio calculations within the framework of the density functional theory in the generalized gradient approximation and of pseudopotential approach. The calculated adsorption energies of the molecules indicate the stepped surface as the most reactive, as expected. The free energy surface during the reaction process has been explored via metadynamics[1]. The optimized configurations of both reactants and products obtained, were then used to accurately calculate the dissociation energy via the Nudge Elastic Band method[2]. [1] A. Laio and M. Parrinello, PNAS 99, 12562 (2002). [2] G. Mills and H. Jonsson, Phys. Rev. Lett. 72, 1124 (1994).

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