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Ethanol adsorption on transition-metal surfaces: A DFT investigation JUAREZ L. F. DA SILVA, Institute of Physics of São Carlos, University of São Paulo, Brazil — The development of low-cost and long-term stability catalyst compounds for the production of hydrogen from ethanol is one of the main problems to be solved for large scale use of direct- ethanol fuel cells. Steam reforming, which is one of the main routes to obtain hydrogen from ethanol, as well as ethanol oxidation, are critically dependent on the choice of the catalyst devices. Therefore, an atom-level understanding of the interaction of ethanol with catalysts systems is on the first problems to be addressed. In this talk, we will report first- principles calculations based on density functional theory for the adsorption of ethanol on close-packed transition-metal surfaces at the limit of low-coverage. In particular, we will report the following properties, namely, adsorption energy, work function changes, and structural parameters for a large number of substrates, which will be used to build up a simple picture to describe the interaction of ethanol with transition-metal surfaces. This work is supported by FAPESP.

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