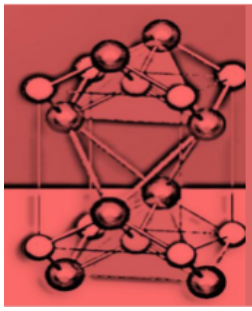

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A theoretical study of ethyl formate adsorption on CaO (001)

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Ethyl formate adsorption on CaO (001) is analyzed using Density Functional Theory (DFT) with Van der Waals corrections, implemented through the Vienna ab Initio Simulation Package (VASP). Our calculations reveals a posible adsorption sites at low coverage with adsorption energies of -1.21 eV, that is more stable than ethanol and less stable than formic acid. Both molecular oxygens bond to two Ca atoms and C methyl bonds to a surface oxygen. The analysis of the electronic structure and bonding show a stabilization of ethyl formate as a result of a shift in their states to lower energies, with respect to the gas phase. A relaxed molecular geometry is obtained after adsorption with no dissociation detected. There is a charge transfer (0.20 e^-) from the adsorbate to the surface. At the same time, H-C (formate) experiment a charge decrease of 0.16 e^-. The Ca-O in the surface shows mostly a decrease in BO after adsorption. In this presentation, we also compare ethyl formate adsorption with previous studies considering formic acid and ethanol in the context of biodisel production.