AB INITIO MOLECULAR DYNAMICS STUDIES OF ETHYLENE GLYCOL PARTIAL OXIDATION ON CO_3O_4(001) SURFACES

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Abstract: The oxidation of 2-propanol to acetone at the Co_3O_4 (001)/H_2O interface has been studied recently, using ab-initio molecular dynamic to understand the role of temperature, surface structure and electrochemical environment [1]. In the same vein, we now study the case of a more complex molecule, namely ethylene glycol, on the same metal oxide surface to understand its oxidation processes. We study the system under dry and humid conditions on the B-terminated surface of Co_3O_4 at room temperature. Under dry conditions, a chemical reaction occurs, when the glycol coverage is increased, and only a deprotonated ethylenedioxy compound is formed as the oxidation product after a simulation time of 20 ps. We then considered the case of a low glycol coverage in presence of up to 3 water molecules and, as expected, more chemical reactions occur (proton exchange and transfer) and concluded that water molecules play a key role in the oxidation of the diol.

Knowing this, we extended these preliminaries studies to a system in liquid water under oxidative conditions (proton deficit and relatively high temperature) for a simulation time of 20 ps. These results will be presented in the contribution.

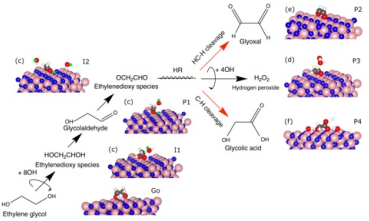

Figure 1: Snapshots of the reaction pathway on the B terminated surface of Co3O4/H2O interface.

[1] Omranpoor, A. H., Kox, T., Spohr, E., & Kenmoe, S. (2022). Influence of temperature, surface composition and electrochemical environment on 2-propanol decomposition at the Co_3O_4 (001)/H2O interface. *Applied Surface Science Advances*, *12*, 100319.