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Mechanistic Study of selective Electrochemical Reduction of Hydroxymethyl Furfural using Grand-Canonical DFT

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Among biomass-platform molecules, 5-hydroxymethylfurfural (HMF) plays an important role since its great potential in the production of industrial monomers, fuels, and pesticides. One of its most interesting products is 2,5-bishydroxymethylfuran (BHMF), that can be used in relevant industrial polymerization processes, such as for polyethers, polyesters and polyamides. In this context, the electrochemical reduction of HMF to BHMF is gaining an increasing interest. The main challenge is to achieve a high faradic efficiency and a good selectivity. Experimentally, it has been shown that using AgCu bimetallic electrocatalysts allowed to achieve a higher conversion, higher selectivity and higher faradic efficiency than the monometallic counter-part.¹

Still, a better understanding of the reaction network is necessary to limit even further the generation of secondary products, in particular humins and to limit the overpotential. Using grand canonical periodic DFT,² we investigated the conversion of HMF into BHMF but also the possible side routes such as the ones yielding to methyl furfural and methyl furfuryl alcohol which involves a C-O scission but also the C-C coupling yielding hydrofuroin, a precursor of humins. This extended reaction network has been explored on Cu, Ag and alloy models surfaces. The competition with the hydrogen evolution reaction³ was also addressed by considering the H coverage in function of the pH and the potential. The influence of the polarization of the electrode is taken into account on the C-C and C-O barrier using a grand canonical approach, which has been shown to be important in cases where the surface dipole induced by the adsorbate is changing during the reaction.⁴

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