Catalyst-free hydrogen synthesis from liquid ethanol: an *ab initio* molecular dynamics study

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Albeit the "*Hydrogen economy*" was proposed almost 50 years ago and notwithstanding the impressive amount of research orbiting around the hydrogen (H_2) production since then, the vast majority of H_2 employed in the energy market stems from steam reforming of hydrocarbons performed at high temperatures (*i.e.*, T ≥ 1000 K). Alternative production channels, such as water and simple alcohols electrolysis *in primis*, have been exploited, allowing for the almost complete elimination of the CO_2 emissions [1]. However, in all cases only by means of costly and rare (*e.g.*, Pt-based, Au-based, biomolecular, etc.) catalysts satisfactory results have been achieved [2,3].

Although up to few years ago electric fields have not been considered as a mean to the chemical synthesis, nowadays a steady growing mass of experimental research is aimed at employing electric fields to finely control chemical reactions [4] and many laboratories have become capable to probe the reactivity-enhancing properties of those fields generated in proximity of emitter tips [5], rendering impelling the extensive usage of electric fields as smart reagents in chemistry [6]. Within this framework, state-of-the-art quantum-based computational approaches represent a benchmark for the experiments. As an example, the field-induced enantioselectivity of specific reactions has been recently investigated by means of sophisticated numerical approaches [7,8]. Moreover, the methanol reaction network under intense electric fields [9,10] has been predicted with these powerful super-computing techniques. Additionally to a brief exploration of the catalytic properties carried by static electric fields, I intend to present a very recent study [11] – based on *ab initio* molecular dynamics simulations – revealing a novel synthesis route to hydrogen from neat liquid ethanol, which has been achieved at room temperature and in absence of any catalyst, upon electric field exposure. The latter result paves the way to the unprecedented catalyst-free experimental synthesis of hydrogen from liquid ethanol by exploiting commonly employed field emitter tips *apparatus*.

References

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