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Application of Periodic DFT Calculation to Catalysis: “Unravelling the Degradation Pathway Facilitating during HMF Oxidation to FDCA over Selected Metals”

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The rising campaign against environmental pollution is discouraging the further exploration of oil and gas^{1,2} while promoting sustainable green and eco-friendly technologies³ is receiving massive attention across the globe in return. 5-Hydroxymethyl furfural (HMF) as a platform molecule in biorefinery with a vast network of derivable products can boost the substitution of existing fossil-based chemicals and fuels with renewable and eco-friendly ones^{1,3}. One of its derivatives is 2,5-furan dicarboxylic acid (FDCA) which is obtainable from a base-free HMF oxidation. Existing literatures^{1,4} has established it to be eco-friendly but suffers a lot of degradation challenges during its usage in FDCA production which is attracting research attention. In search of a solution, we deployed period density functional theory (DFT) calculation to explore the competitive nature of the degradation pathways in contrast with the pathways enhancing HMF oxidation on Au, Pd and Pt using a thermodynamic feasibility study approach.

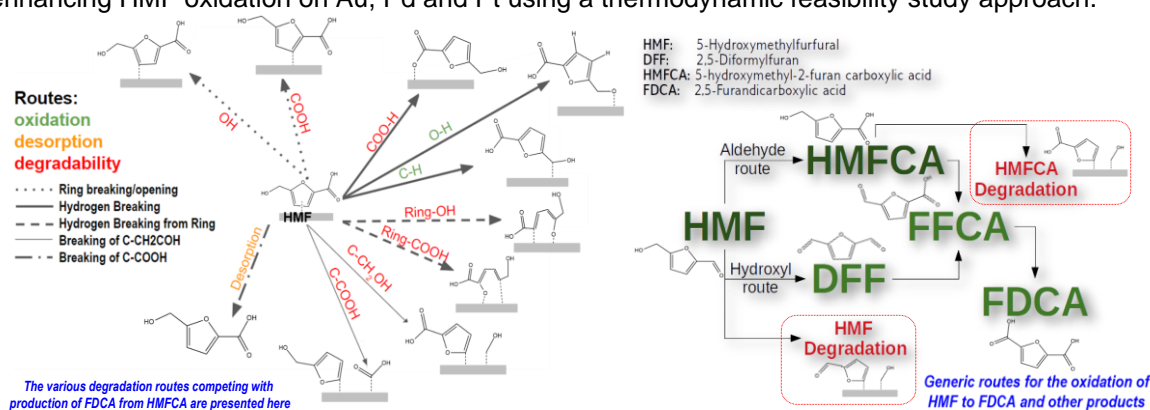


Fig. 1: Scheme of the various HMFOA oxidation and degradation pathways explored.

The study of the species' energy stability (in Fig 1) across respective catalysts for different reaction pathways predicts the HMFOA pathway to be more favourable than 2,5-Diformylfuran (DFF) during FDCA production. The C-CH₂OH scission was identified to be the major degradation route competing with FDCA production across all the catalysts. Au showed the least degradation path while Pt was predicted to have shown the best route for oxidizing HMF to FDCA compared to Pd. Generally, Pt and Au showed better activity and selectivity compared to Pd. The study suggests the design of a new catalyst from the alloying of the respective metals to tap their alloy effects⁵ and complementary advantages in the FDCA production.

- [1] A. D. K. Deshan et al., *Frontiers in Chemistry* **8** (2020) 659.
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- [3] T. Oyegoke, *Bulgarian Chemical Communications* **54** (2022) 29.
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- [5] S. Campisi et al., *J. Carb. Res. C* **4** (2018) 48.