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Selective Oxidation of 3-Hydroxypropionic Acid to Malonic Acid over Pd/C: Mechanistic and Kinetic Study

Background/Objective

- Oxidation of 3-hydroxypropionic acid (3-HP) offers a bio-based pathway to malonic acid (MA), a high-value industrial chemical.
- A combined mechanistic, thermodynamic, and kinetic framework describes the selective oxidation of 3-HP to MA over Pd/C.

Approach

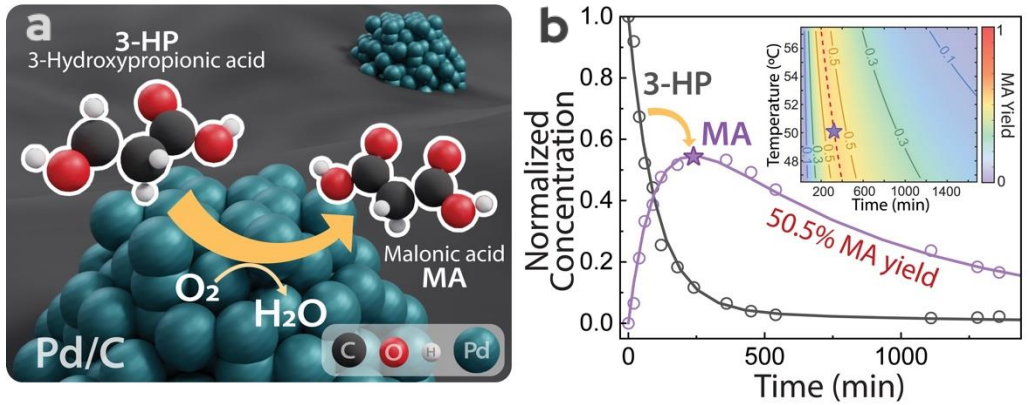
Oxidation data were collected across oxidant loading, pH, and temperature to elucidate reaction trends. Reaction pathways were proposed based on experimental observations and density functional theory (DFT)-calculated thermochemistry. Oxidant-specific kinetic models for O_2 and H_2O_2 were developed.

Results

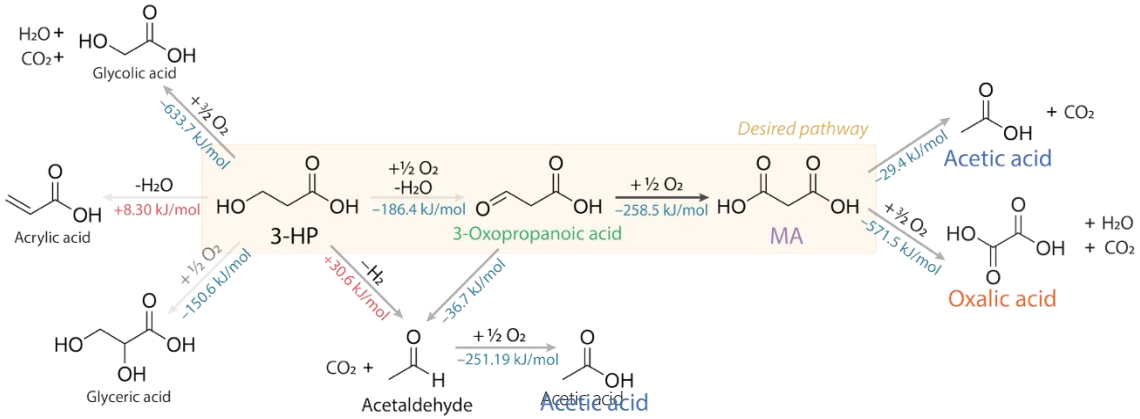
Kinetic models for both oxidants showed excellent agreement with experiment ($R^2 > 0.95$) and revealed distinct behaviors, with O_2 exhibiting superior performance. Optimized conditions for MA production were identified, achieving 56.9% selectivity and 50.5% yield.

Significance/Impacts

The mechanistic and kinetic framework developed here provides a foundation for the selective catalytic production of malonic acid from 3-HP.



(a) Illustration of 3-HP oxidation to MA over Pd/C. (b) Concentration profiles for 3-HP oxidation, with an insert heatmap of MA yield.



A proposed pathway of 3-HP oxidation to MA using O_2 as an oxidant, with DFT-calculated ΔG_{rxn} values are shown for each reaction.

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