

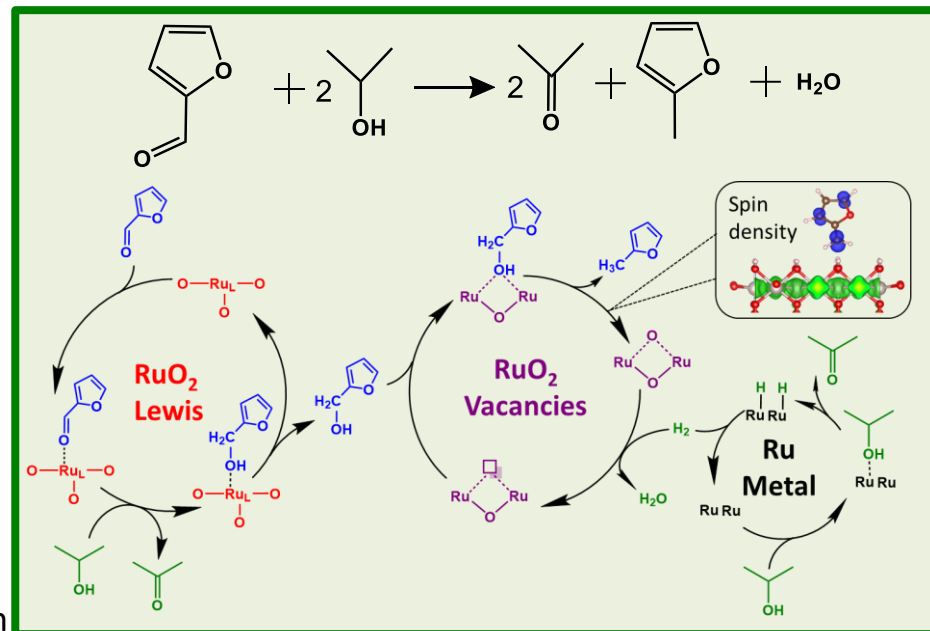
Metal/Metal Oxide Cooperativity for Low-Temperature C-O Bond Activation

Scientific Achievement

Discovered the radical-mediated C-O bond activation mechanism on the multifunctional Ru/RuO_x catalyst that enables up to 76% yield of 2-methyl furan in catalytic transfer hydrogenolysis of furfural using a renewable hydrogen donor.

Significance and Impact

- 2-methyl furan is a renewable drop-in fuel and a versatile platform chemical for jet fuels, lubricants, and aromatics
- Carbon-oxygen bond activation is challenging in biomass-derived compounds due to energy scaling constraints
- Our discovered mechanism and activity factors apply more broadly to various hydrodeoxygenation and ring opening chemistries, providing opportunities for integrated catalyst and reaction pathway design



Research Details

- Selective C-O scission occurs via the conjugation-driven radical mechanism with the reaction barrier of 39 kJ/mol
- RuO₂ vacancies form through a H₂O-like precursor and are active catalytic sites for C-O bond activation
- Catalytic transfer hydrogenolysis of furfural involves three types of catalytic sites: metallic, Lewis acidic, and vacancies
- Unique catalytic properties are due to a conjugation-stabilized furfuryl radical intermediate, strong hydroxyl affinity of RuO₂ oxygen vacancies, and the acid-base heterogeneity of the oxide surface

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Work was performed in CCEI lab at the University of Delaware
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