

## Accepted Manuscript

Title: Oxidative dehydration reaction of glycerol into acrylic acid: A first-principles prediction of structural and thermodynamic parameters of a bifunctional catalyst

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## Highlights

- Oxidative dehydration mechanism of glycerol into acrylic acid is proposed.
- A theoretical analysis of the mechanism was performed using different catalysts.
- The thermodynamic behavior of the reaction was studied.
- The catalyst doped with vanadium presents lower energetic costs during the process.
- The presence of vanadium and peroxy groups produces an active bifunctional catalyst.

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