

AI with experimental and theoretical data: role of the support material for CO₂ hydrogenation

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The performance of heterogeneous catalysts is governed by an intricate interplay of several multi-scale processes. Thus, it is rather challenging to identify the most relevant parameters for the design of the catalyst and its support material. Here, we combine experimental and theoretical descriptive parameters characterizing cobalt nanoparticles dispersed on SiO₂ supports modified with Ti, Zr, Al, Ca, or Mg, and adopt the sure-independence-screening-and-sparsifying (SISSO) AI approach to identify correlations describing the selectivity of these materials measured for the CO₂ hydrogenation to methanol.

Poster title

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