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ORIGINAL PAPER

Application of dual descriptor to understand the activity of Cu/ZrO_2 catalysts in the water gas shift reaction

María Luisa Cerón[1,2] · **Mònica Calatayud**[3,4]

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Abstract A comparative theoretical study applying Dual Descriptor has been performed using Water Gas Shift reaction, catalyzed by copper supported on monoclinic and tetragonal zirconia. The Dual Descriptor and thermodynamic considerations were used to understand the structural effects that occur in the reaction when it is catalyzed by Cu on both zirconia phases. It was found that the formation of carbonates in the Cu supported on tetragonal zirconia dehydrogenates consistently with experimental results.

Keywords Dual descriptor · ZrO_2 · Heterogenous catalysis · WGS · Hydrogen production

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✉ María Luisa Cerón
lceron@uft.cl

[1] Facultad de Ingeniería, Universidad Finis Terrae, Av. Pedro de Valdivia 1509, Providencia, Santiago Chile

[2] Nucleus Millennium Chemical Processes and Catalysis (CPC), Laboratorio de Química Teórica Computacional (QTC), Facultad de Química, Pontificia Universidad Católica de Chile, Casilla 306, Correo 22, Santiago, Chile

[3] Laboratoire de Sorbonne Universités, UPMC Univ Paris 06, CNRS, Laboratoire de Chimie Théorique CC 137 - 4, place Jussieu F. 75252 Paris Cedex 05, France

[4] Institut Universitaire de France, Paris, France