Special Issue

Multi-Scale Modeling of Structured Catalytic Reactors

Message from the Guest Editors

Chemical reactors are the crucial common element in any process that involves conversion. In recent decades, the computational power available for scientific and industrial research has increased significantly, with a simultaneous decrease in the cost of the core-hour. This favorable scenario allowed many research groups to use highly sophisticated computational models to improve our understanding and design of chemical reactors and processes in general. Despite the many advances in the topic over the last decades, there are still many challenges to address to make industrial processes more economically and environmentally attractive. This Special Issue invites significant contributions of multiscale modeling of catalytic reactors, computational models of catalytic substrates, and, especially, in environmental applications. It is hoped that the results published in this Special Issue will contribute to the faster development of the field.

Guest Editors

Dr. Iván Cornejo García

Departamento de Ingeniería Química y Ambiental, Universidad Técnica Federíco Santa Maria, Chile; Department of Chemical and Materials Engineering, University of Alberta, Edmonton, AB T6G 2R3, Canada

Prof. Dr. Robert E. Hayes

Chemical & Materials Engineering Department, University of Alberta, Edmonton, AB T6G 1H9, Canada

Deadline for manuscript submissions

closed (30 September 2021)

Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0
CiteScore 7.6

mdpi.com/si/64022

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
catalysts@mdpi.com

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Prof. Dr. Keith Hohn
Carl R. Ice College of Engineering, Kansas State University, Manhattan, KS, USA

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