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### Descriptors for solid catalysts: 21st century discovery tools

Ras, E.J.

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## Publications

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- “Predicting adsorption on metals: simple yet effective descriptors for surface catalysis”, Erik-Jan Ras, Manuel J. Louwerse, Marjo C. Mittelmeijer-Hazeleger and Gadi Rothenberg, *Phys. Chem. Chem. Phys.*, 2013, 15, 4436-4443
- “New tricks by very old dogs: predicting the catalytic hydrogenation of HMF derivatives using Slater-type orbitals”, Erik-Jan Ras, Manuel J. Louwerse and Gadi Rothenberg, *Catal. Sci. Technol.*, 2012, 2, 2456-2464
- “The High-throughput research approach to biorefineries—A powerful tool for studying the complexity of catalytic processes”, Jan-Kees van der Waal, Robert-Jan van Putten, Erik-Jan Ras, Martin Lok, Gert-Jan Gruter, Marjolein Brasz and Ed de Jong, *Cellulose Chem. Technol.*, 2011, 45 (7-8), 461-466
- “Understanding catalytic biomass conversion through data mining”, Erik-Jan Ras, Ben McKay and Gadi Rothenberg, *Topics in Catalysis*, 2010, 53 (15-18) 1202-1208
- “Selective Hydrogenation of 5-Ethoxymethylfurfural over Alumina-Supported Heterogeneous Catalysts”, Erik-Jan Ras, Sergio Maisuls, Paul Haesakkers, Gert-Jan Gruter and Gadi Rothenberg, *Adv. Synth. Catal.*, 2009, 315(18), 3175-3185
- “Prediction of Maximum Yield in the Crystallization of Multicomponent Isomeric Systems”, Alan A. Smith, Ben McKay, Eric W. P. Damen, Simone Darphorn-Hooijschuur, Erik-Jan Ras, and Goran Verspui, *Org. Process Res. Dev.*, 2006, 10 (6), 1132–1143
- “Asymmetric Catalytic Ketone Hydrogenation: Relating Substrate Structure and Product Enantiomeric Excess Using QSPR”, Johannes B. van der Linden, Erik-Jan Ras, Simone M. Hooijschuur, Guido M. Klaus, Niels T. Luchters, Paulo Dani, Göran Verspui, Alan A. Smith, Eric W. P. Damen, Ben McKay, Marcel Hoogenraad, *QSAR & Comb. Sci.*, 2005, 24 (1), 94-98

Several patents were filed by Siluria Technologies where the author is listed as co-inventor. The underlying research that led to these patent applications was performed using the methodology described in this manuscript:

- “Catalysts for petrochemical catalysis”, WO2012162526A2
- “Nanowire catalysts and methods for their use and preparation”, WO2013082318A2