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Progress and perils in predictive computational catalysis

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D202 Seminar room, School of Engineering, 2nd Floor

Abstract: In recent work [J. Chem. Phys., 143, 094106 (2015)], we have proposed a novel computational strategy, path-constrained molecular dynamics (PCMD), for automated sampling of chemical reaction paths. In this seminar, I will show how PCMD can be used to construct kinetic models for complex chemical systems; interrogation of these kinetic models enables extraction of properties such as rate laws and mechanisms. I will highlight new results which demonstrate how PCMD and kinetic modelling can be applied to direct elucidation of the reaction mechanism of a catalytic cycle, namely cobalt-catalysed hydroformylation of ethene; while these results are the first-ever demonstration of an automated approach to predictive catalysis, I will also highlight the role of errors and uncertainty in our computational approach.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars

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