THE OHIO STATE UNIVERSITY

The William G. Lowrie Department of Chemical and Biomolecular Engineering Graduate Program

Cordially invites you to attend a seminar on

The degree of rate control:
a powerful tool for catalysis research

Charles T. Campbell
The B. Seymour Rabinovitch Endowed Chair
in Chemistry
Chemistry Department
University of Washington

Thursday, October 24, 1:30 PM
110-120 Koffolt Lab
CBEC 151 W Woodruff Ave
Reception at 1:00 pm in 110-120 CBEC

Bio

Prof. Charles T. Campbell is the Rabinovitch Endowed Chair in Chemistry at the University of Washington, where he is also Adjunct Professor of Chemical Engineering and of Physics. He is the author of over 330 publications and two patents on surface chemistry, catalysis, physical chemistry and biosensing, with over 27,000 total citations and an h-index of 88 (Google Scholar). He is an elected Fellow of the ACS, the AVS and the AAAS, and Member of the Washington State Academy of Sciences. He received the Arthur W. Adamson Award of the ACS and the ACS Award for Colloid or Surface Chemistry, the Gerhard Ertl Lecture Award, the Robert Burwell Award/Lectureship of the North American Catalysis Society, the Medard W. Welch Award of the AVS, the Gauss Professorship of the Göttingen Academy of Sciences, the Ipatieff Lectureship of Northwestern University and an Alexander von Humboldt Research Award. He served as Editor-in-Chief of *Surface Science* for over ten years, and now serves as Editor-in-Chief of *Surface Science Reports*, and on the Boards of *Catalysis Reviews*, *Catalysis Letters* and *Topics in Catalysis*. He received his BS (1975) and PhD (1979) degrees at the University of Texas at Austin in Chemical Engineering and Chemistry, respectively, then did postdoctoral research in Germany under Gerhard Ertl (who won the 2007 Nobel Prize in Chemistry).

Abstract

The "degree of rate control" (DRC) is a mathematical approach for analysing multi-step reaction mechanisms that has proven very useful in catalysis research.[1] It identifies the "rate-controlling transition states and intermediates" (i.e., those whose DRCs are large in magnitude). Even in mechanisms with over 30 intermediates and transition states, these are generally just a few distinct chemical species whose energies, if they could be independently changed, would achieve a faster net reaction rate to the product of interest. For example, when there is a single "rate-determining step", the DRC for its transition state (TS) is 1, and the DRC for other TSs is zero (if a series reaction). Since the (relative) energies of these key adsorbed intermediates and transition states can be adjusted by modifying the catalyst or solvent, or even a reactant's molecular structure, the DRC values provide important ideas for catalyst improvement. The species with large DRCs are also the ones whose energetics must be most accurately measured or calculated to achieve an accurate kinetic model for any reaction mechanism. A tutorial on DRC analysis is presented here. Applications of DRC analysis include:[1] clarifying reaction kinetics, predicting and interpreting apparent activation energies,[2] improving the accuracy of computational microkinetic models, high-throughput computational screening of catalyst materials, improving reaction conditions, improving choice of oxidant in selective oxidation, and explaining kinetic isotope effects. Since DRC values can be determined experimentally, a full microkinetic model is not required to take advantage of DRC analysis.

References:

1. C. T. Campbell, *ACS Catalysis* 7 (2017) 2770.

2. Z. T. Mao and C. T. Campbell, *ACS Catalysis* 9 (2019) 9465.

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