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EPFL Valais/Wallis SEMINAR

11. 11. 2020, 17:00-18:00, EPFL Valais/Wallis ZOOM Seminar

Oxide-supported metal nanoparticles: predicting how size and support affect metal atom energetics and thus catalytic performance

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Many important catalysts and electro-catalysts for energy and environmental technologies involve late transition metal nanoparticles dispersed across the surface of some oxide support. The activity and long-term stability of these materials depend strongly on particle size below 5 nm, and, in this size range, upon the nature of the oxide support. The relationships between the energetic stability of late transition metal particles on oxide supports and their structural, electronic, chemisorption and catalytic properties have been examined in detail. We derived a quantitative equation that predicts the energy of the metal atoms in these nanoparticles (i.e., the metal-atom chemical potential, as measured by metal vapor adsorption calorimetry) and their particle size as well as their adhesion energy to the oxide surface (Eadh), and improved it with an empirical correction factor. Furthermore, measurements of the metal / oxide adhesion energy reveal that Eadh increases with: (1) increasing oxophilicity of the metal (estimated from the heat of formation of the oxide of the metal from metal gas plus O2, (2) decreasing oxophilicity of the oxide support (estimated from the heat of reduction of the metal oxide support to its next lower oxide), and (3) increasing density of coordinatively-unsaturated O atoms on the surface of the oxide. The strength with which oxide-supported metal particles bond adsorbates, their catalytic kinetics and their sintering rates also correlate with this metal-atom chemical potential. Thus, these results help explain particle size and support effects in catalysis.

Work supported by DOE-OBES Chemical Sciences Division.

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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 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). He is the author of over 330 publications and two patents on surface chemistry, catalysis, physical chemistry and biosensing, with over 29,000 total citations and an h-index of 90 (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, the ACS Award for Colloid or Surface Chemistry, the ACS Catalysis Award for Exceptional Achievements, 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*.