Preface

Ewa Brocławik · Dorota Rutkowska-Zbik ·
Renata Tokarz-Sobieraj

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This issue of Structural Chemistry is dedicated to Professor Małgorzata Witko on the occasion of her anniversary and collects contributions from her friends in science, sharing common interests and, at times, collaborating with Professor Witko.

Professor Małgorzata Witko was born in Cracow, Poland. She graduated with M.Sc. in Chemistry from the Jagiellonian University in Cracow (1973) and with Ph.D. in Theoretical and Physical Chemistry from the Institute of Physical Chemistry, Polish Academy of Sciences in Warsaw (1978). Her entire professional career was connected with the Institute of Catalysis and Surface Chemistry (ICSC), now the Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences. Professor Małgorzata Witko was awarded the degree of D.Sc. in Theoretical and Physical Chemistry from the Jagiellonian University (1991) and in 1997 she culminated with the title of Professor. Since 2002, she has been the Director of The Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences. In 2007, she has been elected to be a member of the Polish Academy of Sciences.

Throughout her scientific career, Professor Małgorzata Witko has published over 130 papers, among which one finds the first scientific paper in which catalytic phenomena are approached by theoretical methodology. She is an author of two sections in handbooks: “Theoretical Aspects of Molecular Catalysis”, in *Education in Advanced Chemistry* (1995) and “Theory of Physical and Chemical Behavior of Transition Metal Oxides: Vanadium and Molybdenum Oxides”, in series entitled “The Chemical

Physics of Solid Surfaces” (2001). In the recognition of her expertise in this field, she was invited to serve as Guest Editor by many scientific journals: *Journal of Molecular Catalysis* (54 (3)/1989, 82 (2–3)/1993, 166/2001), *Topics in Catalysis* (11–12/2000, 169/2011), *Applied Surface Science* (252(3)/2005), “Metal–Ligand Interactions” NATO Science Series II. Mathematics, Physics and Chemistry (V. 116, 2003). She spent her post-doc in the Université Paris-Sud, CNRS, Orsay (1980/81). She was awarded Alexander von Humboldt Fellow and she stayed 1.5 years in 1992–1993 and 4 months in 1998 in Fritz-Haber Institute MPG, Berlin. Professor Witko was also invited as a Visiting Professor by numerous universities: Université Paris-Sud, CNRS, Orsay, France (in 1977, 1980, 1981), Freie Universität, Berlin (in 1981, 1982, 1983, 1984, 1985, 1986), The National Research Council, Italy (in 1989). She established wide national and international collaboration with many respected scientific institutions: Fritz-Haber-Institut der MPG, Berlin, Germany (since 1992), Faculty of Chemistry, Jagiellonian University, Krakow, Poland (since 1998), Laboratory of Microbial Biochemistry, Fachbereich Biologie, Philipps-Universität Marburg, Germany (since 2003), Institut für Materialphysik, University of Wien, Austria (since 2002), Laboratoire de Chimie Théorique, Université Pierre et Marie Curie in Paris, France (since 2003).

Entering the Institute of Catalysis with theoretical background, she quickly developed strong interests in the field of heterogeneous, homogeneous, and enzymatic catalysis. In *heterogeneous catalysis*, her research has been focused on the electronic structure of transition metal oxides, mostly vanadium- and molybdenum-based ones, including binary (V_2O_5 , VO_2 , V_2O_3 , MoO_3 , MoO_2), mixed ($V-O-P$, $Mg-O-V$, $Mo-O-Co$, $Mo-O-Ni$, $Mo-O-Bi$), alkali-doped systems, as well as supported on oxide-type

E. Brocławik · D. Rutkowska-Zbik · R. Tokarz-Sobieraj (✉)
Jerzy Haber Institute of Catalysis and Surface Chemistry,
Polish Academy of Science, Kraków, Poland
e-mail: nctokarz@cyf-kr.edu.pl

materials (SiO_2 , Al_2O_3 , and TiO_2). The main achievements in Professor Witko's original field are: explanation of the differences in thermodynamic stability and catalytic activity of various low-index crystallographic planes exposed during a catalytic reaction, investigation of structurally different oxygen and metal centers, description of surface vacation formation and re-oxidation processes, explanation of the role of oxygen vacancies as active centers, investigation of the hydrogen behavior on oxide surfaces (migration, formation of surface hydroxyl and water species, formation of bronzes).

Małgorzata Witko is recognized not only as a scientist but also as a tutor of young researchers. Based on her own alumni, she established a strong group specializing in molecular modeling of catalytic processes and opening new areas of expertise. The research in the field of *homogeneous catalysis* has covered mainly theoretical modeling of catalytic activity of porphyrins. The main achievements here are: the description of binding and activation of molecular oxygen leading to the formation of manganese oxoporphyrin, elucidation of the mechanism of epoxidation of cyclohexene by manganese porphyrin, modeling of oxidation of cyclohexene to cyclohexene alcohol over manganese porphyrin. The studies in *enzymatic catalysis* have been focused on ethylbenzene dehydrogenase (EBDH), the enzyme catalyzing stereospecific hydroxylation of ethylbenzene to (S)-1-phenylethanol. The main achievements in that area are: the detailed description of molecular mechanism of ethylbenzene oxidation to +(S)-1-phenylethanol and development of the theoretical multiple regression model, which relates experimentally measured kinetic constants to the theoretical and experimental electronic and steric parameters.

Małgorzata Witko is a member of many scientific societies and professional organizations such as the Polish Chemical Society (since 1973, for which she served as a member of executive board of Theory Section from 2001 to 2004, later as a member of executive board of Krakow Section in 2006–2008, and finally as a member of Presidium of the Polish Chemical Society from 2010 until now), Polish Catalysis Club (since 1994), the European Federation of Catalysis Societies (polish delegate and Vice President in 2005–2009), Committee of Chemistry of the

Polish Academy of Sciences, member of panel V of the European Research Council. She is a member of the scientific boards of two institutions: the Institute of Physical Chemistry and the Institute of Nuclear Physics, Polish Academy of Sciences.

Professor Małgorzata Witko was the main organizer of numerous international conferences, among which International Conference “Catalysis for Society” (2008), International Symposium “Catalysis on Oxide-Type Materials. Theory and Experiment: Share Needs and Capabilities” (2005), 3rd EFCATS School on Catalysis (2004), International Conference on Theoretical Aspects of Catalysis (1992, 2002), International Symposium “Catalysis in XXI Century: From Quantum Chemistry to Industry” (2000) were the most significant. Her expertise in theory and catalysis has been further recognized by frequent invitations to Organizing Committees and Advisory Boards of congresses, conferences and symposia. She has given more than 100 invited and plenary lectures, contributing to understanding problems of theoretical chemistry and catalysis. During last 3 years, she actively participated in 27th International Conference “Neutron Scattering Spectroscopy and Related Problems” (Poland, 2011), “Marie Skłodowska-Curie Symposium on the Foundation of Physical Chemistry” (Poland, 2011), 13 International Conference of Theoretical Aspects of Catalysis (Japan, 2010), i-CATs Innovation in Catalysis for Sustainable Production & Energy. Towards a roadmap for catalysis (Italy, 2010), The Seventh International Symposium Effect of Surface Heterogeneity in Adsorption and Catalysis (Poland, 2009), Conference on Nanocatalysis: Fundamentals & Applications (China, 2008), to name but a few.

Professor Witko is the holder of the Knight's Cross of the Order of Polonia Restituta (2011). She is well known as a woman scientist who manages to successfully join professional and private life with her great passion for good music, literature, and travelling.

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