

**Dr. Stefan Vajda***Senior Chemist*

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Research Summary:

- Atomically precise clusters and cluster-based materials
- Nanocatalysis: Study of the cluster size/composition & function relationship at the sub-nanometer and nanometer scale, support effects in catalysis
- Electrocatalysis by clusters (water oxidation, CO₂ conversion)
- Clusters and cluster-based assemblies in Li-O₂ electrochemistry
- CO₂ and CO conversion; selective catalysis under low pressure and at low temperature
- Combined *in situ* synchrotron X-ray scattering, X-ray absorption and mass-spectroscopy studies of nanocatalysts under realistic reaction conditions

Professional Preparation

1980-1985 M.Sc. Physical Chemistry, Charles University Prague, Czechoslovakia
1985-1989 Ph.D. Chemistry Charles University Prague, Czechoslovakia
1991-1992 Fulbright Fellow, The University of Chicago
2000-2002 Habilitation – University Teaching Qualification (Experimental Physics)
Freie Universität Berlin, Germany

Graduate advisor: V. Fidler**Postdoctoral advisor:** G. R. Fleming**Habilitation advisor:** L. Wöste**Professional Experience**

2011-present Senior Chemist, Materials Science Division, Argonne
2013-2016 Institute for Molecular Engineering (IME) Fellow, The University of Chicago
2007-2016 Adjunct Full Professor, Department of Chemical & Environmental Engineering, Yale University
2006-2016 Joint appointment with the Center of Nanoscale Materials, Nanoscience & Technology Division, Argonne National Laboratory
2010-2011 Chemist, Materials Science Division, Argonne
2007-2011 Chemist, Chemical Sciences and Engineering Division, Argonne
2002-2007 Chemist, Chemistry Division, Argonne
2000-2002 University Senior Assistant (C1), Institut für Experimentalphysik, Freie Universität Berlin, Germany
1995-2000 Researcher, project leader, Institut für Experimentalphysik, Freie Universität Berlin
1992-1995 Researcher, Department of Chemical Physics Charles University Prague
1992-1995 Researcher, Department of Physical Chemistry, Charles University Prague
1991-1992 Fulbright Fellow, Department of Chemistry, The University of Chicago
1989-1991 Researcher, Departments of Physical Chemistry, Charles University Prague

Recent Professional Activities

- Discussion leader, Gordon Research Conference, Clusters and Nanostructures (2017)
- Guest Editor, with Alessandro Fortunelli, *Cat. Sci.Tech.*, Topical Issue “Nanocatalysis” (2016)
- Guest Editor, with Jeroen van Bokhoven, *Phys. Chem. Chem. Phys.*, Topical Issue “Size Selected Clusters and Particles: From Physical Chemistry to Catalysis” (2014)
- Conference organizer, Cluster-Surface Interactions Workshop 2016
- Symposium organizer, Catalytic Materials for Energy and Sustainability, 2016 MRS Fall Meeting
- Symposium organizer, Symposium on Catalytic Materials for Energy, 2015 MRS Fall Meeting
- Discussion Symposium organizer and Co-Chair, XIth European Congress on Catalysis (2013)
- Discussion leader, Gordon Research Conference, Gaseous Ions: Structures, Energetics and Reactions, session “From Ions to Nanomaterials” (2013)
- Coordinator with Lisa Pfefferle of a Yale-based AFOSR MURI project (2008-2013)
- Proposal Study Panel of the Advanced Light Source, LBNL (since 2011)

Selected recent publications (total publications – over 100)

1. “Alumina-Supported Sub-nanometer Pt₁₀ Clusters: Amorphization and Role of the Support Material in a Highly Active CO Oxidation Catalyst”, C. Yin, F. R. Negreiros, G. Barcaro, A. Beniya, L. Sementa, E. C. Tyo, S. Bartling, K.-H. Meiwes-Broer, S. Seifert, H. Hirata, N. Isomura, S. Nigam, C. Majumder, Y. Watanabe, A. Fortunelli, and S. Vajda, *J. Mater. Chem. A* **5**, 4923 (2017)
2. “Water Oxidation by Size Selected Co₂₇ Clusters Supported on Fe₂O₃”, M. J. Pellin, S. C. Riha, E. C. Tyo, G. Kwon, J. A. Libera, J. W. Elam, S. Seifert, S. Lee, and S. Vajda, *ChemSusChem*. **9**, 3005 (2016)
3. “Electrochemical Behaviour of Naked Sub-Nanometre Sized Copper Clusters and Effect of CO₂”, R. Passalacqua, S. Parathoner, G. Centi, A. Halder, E. C. Tyo, B. Yang, S. Seifert and S. Vajda, *Catal. Sci.Technol.* **6**, 6977 (2016)
4. “Catalysis by Clusters with Precise Number of Atoms”, E. C Tyo and S. Vajda, *Nat. Nano.* **10**, 577 (2015), *invited review*
5. “Carbon Dioxide Conversion to Methanol over Size-selected Cu₄ Clusters at Low Pressures”, C. Liu, B. Yang, E. Tyo, S. Seifert, J. E. Ernst, B. von Issendorff, P. Zapol, S. Vajda and L. A. Curtiss, *J. Am. Chem. Soc.* **137**, 8676 (2015)
6. “Fischer–Tropsch Synthesis at a Low Pressure on Subnanometer Cobalt Oxide Clusters: The Effect of Cluster Size and Support on Activity and Selectivity”, S. Lee, B. Lee, S. Seifert, R.E. Winans and S. Vajda, *J. Phys. Chem. C* **119**, 11210 (2015)
7. “Effect of the Size-Selective Silver Clusters on Li₂O₂ Morphology in Lithium-Oxygen Batteries”, J. Lu, L. Cheng, K.C. Lau, E. C. Tyo, X. Luo, J. Wen, D. Miller, R. Assary, H.H. Wang, P. Redfern, H. Wu, J.B. Park, Y.K. Sun, S. Vajda, K. Amine, L. A. Curtiss, *Nat. Commun.*, 5895 (2014)
8. “Size-Dependent Subnanometer Pd Clusters (Pd₄, Pd₆, and Pd₁₇) Water Oxidation Electrocatalysis”, G. Kwon, E. C. Tyo, C. Yin, G. A. Ferguson, J. DeBartolo, S. Seifert, R. E. Winans, A. J. Kropf, C. J. Heard, R. L. Johnston, J. P. Greeley, L. A. Curtiss, M. J. Pellin, and S. Vajda, *ACS Nano* **7**, 5808 (2013)
9. “Increased Silver Activity for Direct Propylene Epoxidation via Subnanometer Size Effects”, Y. Lei, F. Mehmood, S. Lee, J. P. Greeley, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, R. J. Meyer, P. C. Redfern, D. Teschner, R. Schlögl, M. J. Pellin, L. C. Curtiss, and S. Vajda, *Science* **328**, 224 (2010)
10. “Selective Propene Epoxidation on Immobilized Au₆₋₁₀ Clusters: The Effect of Hydrogen and Water on Selectivity and Activity”, S. Lee, L. M. Molina, M. L. María J. López, J. A. Alonso, B. Hammer, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, M. J. Pellin, and S. Vajda, *Angew. Chemie Int. Ed.* **48**, 1467 (2009)
11. “Subnanometer Platinum Clusters as Highly Active and Selective Catalysts for the Oxidative Dehydrogenation of Propane”, S. Vajda, M. J. Pellin, J. P. Greeley, C. L. Marshall, L. A. Curtiss, G. A. Ballentine, J. W. Elam, S. Catillon-Mucherie, P. C. Redfern, F. Mehmood and P. Zapol, *Nat. Mater.* **8**, 213 (2009)

Complete List of Publications

I.	Publications in refereed journals & refereed book chapters	2
II.	Publications in journals (not refereed papers)	13
III.	Publications in conference proceedings	13
IV.	Publications - preprints	15
V.	Publications in books of abstracts - extended reviewed abstracts	16

Summary

Publications: around 100, including one in *Angewandte Chemie*, *Journal of the American Chemical Society*, *Nature Materials*, *Nature Communications* and *Nature Nanotechnology*; two in *Nano Letters*, *Physical Review Letters* and *Science*; three in *ACS Nano*.

Select highly cited papers: *Science* (2003), *Angewandte Chemie* (2009), *Nature Materials* (2009), *Science* (2010), *ACS Nano* (2013), *Nature Nanotechnology* (2015)

Editors' Choice: *J. Chem. Phys.* 2009, *Phys. Chem. Chem. Phys.* 2011

I. Publications in refereed journals & refereed book chapters

- I-97.** “Copper Cluster Size Effect in Methanol Synthesis from CO₂ “
B. Yang, C. Liu, A. Halder, E. C. Tyo, A. B.F. Martinson, S. Seifert, P. Zapol, L. A. Curtiss, S. Vajda
J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.7b01835, published on line May 8, 2017, [link](#)
- I-96** “Anomalous Diffusion of a Single-Atom Metal Catalyst on a Graphene Oxide Support”
T. Furnival, R. K. Leary, E. C. Tyo, S. Vajda, Q. M. Ramasse, J. Meurig Thomas, P. D. Bristowe, P. A. Midgley
Chem. Phys. Lett. DOI: 10.1016/j.cplett.2017.04.071, published on-line April 21, 2017, *invited paper*, [link](#)
- I-95.** “Size-Selective Reactivity of Ag₄ vs Ag₁₆ with CO on TiO₂ Surface“
P.-T. Chen, E. C. Tyo, M. Hayashi, M. J. Pellin, M. Nachtegaal, O. Safonova, J. van Bokhoven, L.-C. Chen, S. Vajda, and P. Zapol
J. Phys. Chem. C, **121**, 6614–6625 (2017), DOI: 10.1021/acs.jpcc.6b11375, [link](#)
- I-94.** “Alumina-Supported Sub-nanometer Pt₁₀ Clusters: Amorphization and Role of the Support Material in a Highly Active CO Oxidation Catalyst”
C. Yin, F. R. Negreiros, G. Barcaro, A. Beniya, L. Sementa, E. C. Tyo, S. Bartling, K.-H. Meiwes-Broer, S. Seifert, H. Hirata, N. Isomura, S. Nigam, C. Majumder, Y. Watanabe, A. Fortunelli, and S. Vajda
J. Mater. Chem. A **5**, 4923-4931 (2017), DOI: 10.1039/C6TA10989F, [link](#)
- I-93.** “Bandgap Inhomogeneity of a PbSe Quantum Dot Ensemble from Two-Dimensional Spectroscopy and Comparison to Size Inhomogeneity from Electron Microscopy”
S. Park, D. Baranov, J. Ryu, B. Ch, A. Halder, S. Seifert, S. Vajda, and D. Jonas
Nano Letters **17**, 562-571 (2017), DOI: 10.1021/acs.nanolett.6b03874, [link](#)
- I-92.** “Modification of Gas Aggregation Sources: High Pressure and Reactive Gas Magnetron Sputtering”
L. Kolipaka and S. Vajda
in “*Gas Phase Synthesis of Nanoparticles*”, Wiley-VCH, Ed.: Y. Huttel, Chapter 2, ISBN: 978-3-527-34060-6, accepted in March 2016, Ebook published in March 2017, book to be published in April 2017, *invited chapter*, [link](#)
- I-91.** “Water Oxidation by Size Selected Co₂₇ Clusters Supported on Fe₂O₃”
M. J. Pellin, S. C. Riha, E. C. Tyo, G. Kwon, J. A. Libera, J. W. Elam, S. Seifert, S. Lee, and S. Vajda
ChemSusChem. **9**, 3005-3011 (2016), DOI: 10.1002/cssc.201600982, [link](#)
- I-90.** “Temperature-Dependent Evolution of the Oxidation States of Cobalt and Platinum in Co_{1-x}Pt_x Clusters under H₂ and CO + H₂ Atmospheres”
B. Yang, G. Khadra, J. Tuaille-Combes, E. C. Tyo, M.J. Pellin, B. Reinhart, S. Seifert, X. Chen, V. Dupuis, S. Vajda
J. Phys. Chem. C **120**, 21496–21504 (2016), DOI: 10.1021/acs.jpcc.6b06483, [link](#)

- I-89.** “Editorial: Nanocatalysis”
A. Fortunelli and S. Vajda
Catal. Sci. Technol. **6**, 6763–6765 (2016), DOI: 10.1039/c6cy90085b, *invited paper & journal front cover*, [link](#)
- I-88.** “In Situ Study of the Electronic Structure of Atomic Layer Deposited Oxide Ultrathin Films upon Oxygen Adsorption Using Ambient Pressure XPS”
B.H. Mao, E. Crumlin, M. J. Pellin, E. C. Tyo, S. Vajda, Y. Li, S.-D. Wang, and Zhi Liu
Catal. Sci. Technol. **6**, 6778–6783 (2016), DOI: 10.1039/c6cy00575f, *invited paper*, [link](#)
- I-87.** “Electrochemical Behaviour of Naked Sub-Nanometre Sized Copper Clusters and Effect of CO₂”
R. Passalacqua, S. Parathoner, G. Centi, A. Halder, E. C. Tyo, B. Yang, S. Seifert and S. Vajda
Catal. Sci. Technol. **6**, 6977–6985 (2016), DOI: 10.1039/c6cy00942e, *invited paper*, [link](#)
- I-86.** “Atomistic and Electronic Structure Methods for Nanostructured Oxide Interfaces”
G. Barcaro, L. Sementa, F. Ribeiro Negreiros, I. O. Thomas, S. Vajda, A. Fortunelli
in “*Oxide Materials at the Two-dimensional Limit*”, Springer Series in Materials Science, Springer, Eds: F. P. Netzer and A. Fortunelli, Chapter 2, pp. 39–90 (2016) DOI 10.1007/978-3-319-28332-6-2, *invited chapter*, [link](#)
- I-85.** “Catalysis Applications of Size-selected Cluster Deposition”
S. Vajda and M.G. White
ACS Catalysis **5**, 7152–7176 (2015), DOI: 10.1021/acscatal.5b01816, *invited perspective*, [link](#)
- I-84.** “Catalysis by Clusters with Precise Number of Atoms”
E. C Tyo and S. Vajda
Nat. Nanotech. **10**, 577–588 (2015), DOI: 10.1038/nnano.2015.140, *invited review*, [link](#)
- I-83.** “Carbon Dioxide Conversion to Methanol over Size-selected Cu₄ Clusters at Low Pressures”
C. Liu, B. Yang, E. Tyo, S. Seifert, J. E. Ernst, B. von Issendorff, P. Zapol, S. Vajda and L. A. Curtiss
J. Am. Chem. Soc. **137**, 8676–8679 (2015), DOI: 10.1021/jacs.5b03668, *Communication*, [link](#)
- I-82.** “Pronounced Size Dependence in Structural and Morphological Transitions of Gas-Phase Produced and Partially Oxidized Co Nanoparticles under Catalytic Reaction Conditions”
S. Bartling, C. Yin, I. Barke, K. Oldenburg, H. Hartmann, V. von Oeynhausen, M.-. Pohl, K. Houben, E. C. Tyo, S. Seifert, P. Lievens, K.-H. Meiwes-Broer and S. Vajda
ACS Nano **9**, 5984–5998, (2015), DOI: 10.1021/acsnano.5b00791, [link](#)
- I-81.** “Fischer–Tropsch Synthesis at a Low Pressure on Subnanometer Cobalt Oxide Clusters: The Effect of Cluster Size and Support on Activity and Selectivity”
S. Lee, B. Lee, S. Seifert, R.E. Winans and S. Vajda
J. Phys. Chem. C **119**, 11210–11216 (2015), DOI: 10.1021/jp512157d, *invited article*, [link](#)

- I-79.** “Editorial: Size-Selected Clusters and Particles: From Physical Chemistry and Chemical Physics to Catalysis“
J. A. Van Bokhoven and S. Vajda
Phys. Chem. Chem. Phys. **16**, 26418-26420 (2014), DOI: 10.1039/c4cp90163k, [link](#)
- I-78.** “Ambient pressure XPS study of silver clusters on Al₂O₃ and TiO₂ ultrathin film supports”
B. H. Mao, R. Chang, L. Shi, Q. Q. Zhuo, S. Rani, X. S. Liu, E. C. Tyo, S. Vajda, S. D. Wang, and Z. Liu
Phys. Chem. Chem. Phys. **16**, 26645-26652 (2014), DOI: 10.1039/c4cp02325k , *invited article*, [link](#)
- I-77.** “Physical Fabrication of Nanostructured Heterogeneous Catalysts”
C. Yin, E. C. Tyo and S. Vajda
Chapter 3 in “*Heterogeneous Catalysis at the Nanoscale for Energy Applications*”, Eds. F. Tao, W. Schneider, and P. Kamat, Wiley-VCH, ISBN 0470952601, ISBN 978-0470952603 (December 2014) , *invited chapter*, [link](#)
- I-76.** “Effect of the Size-Selective Silver Clusters on Li₂O₂ Morphology in Lithium-Oxygen Batteries”
J. Lu, L. Cheng, K.C. Lau, E. C. Tyo, X. Luo, J. Wen, D. Miller, R. Assary, H.H. Wang, P. Redfern, H. Wu, J.B. Park, Y.K. Sun, S. Vajda, K. Amine, L. A. Curtiss
Nat. Commun., 5895 (2014), DOI: 10.1038/ncomms5895, [link](#)
- I-75.** “Pd_nAg_(4-n) and Pd_nPt_(4-n) clusters on MgO (100): A density functional surface genetic algorithm investigation”
C. J. Heard, S. Heiles, S. Vajda and R. L. Johnston
Nanoscale **6**, 11777–11788 (2014), DOI: 10.1039/c4nr03363a, [link](#)
- I-74.** “Atomically Precise (Catalytic) Particles Synthesized by a Novel Cluster Deposition Instrument“
C. Yin, E. Tyo, K. Kuchta, B. von Issendorff, and S. Vajda
J. Chem. Phys. **140**, 174201-1-7 (2014), DOI: 10.1063/1.4871799, [link](#)
- I-73.** “Support and Oxidation Effects on Subnanometer Palladium Nanoparticles”
C. J. Heard, S. Vajda, R. L. Johnston
J. Phys. Chem C **118**, 3581-3589 (2014), DOI: 10.1021/jp411019t, [link](#)
- I-72.** “Size and Support Dependent Evolution of the Oxidation State and Structure by Oxidation of Subnanometer Cobalt Clusters”
C. Yin, F. Zheng, S. Lee, J. Guo, W.C. Wang, G. Kwon, V. Vajda, H. Wang, B. Lee, J. DeBartolo, S. Seifert, R. E. Winans, and S. Vajda
J. Phys. Chem. A **118**, 8477–8484 (2014), DOI: 10.1021/jp501817u, [link](#)
- I-71.** “Reaction Mechanism for Direct Propylene Epoxidation by Alumina-Supported Silver Aggregates: The Role of the Particle / Support Interface”
L. Cheng, C. Yin, F. Mehmood, B. Liu, J. P. Greeley, S. Lee, B. Lee, S. Seifert, R. E. Winans , D. Teschner, R. Schlögl, S. Vajda, L. A. Curtiss

- ACS Catal.* **4**, 32–39 (2014), DOI: 10.1021/cs4009368, [link](#)
- I-70.** “Ultrafast Dynamics & Control: From Electronic State Population Control to Selective Bond Breaking”
S. Vajda, and L. Wöste
in *The Dekker Encyclopedia of Nanoscience and Nanotechnology Third Edition*, Ed.: S.E. Lyshevski, *Third Edition*. CRC Press: New York, 2014, pp. 4560–4574. *invited review entry*, [link](#)
- I-69.** “Oxidation of Cyclohexane by Size-Selected Palladium Clusters Pinned in Graphite: Cluster Stability and Identification of the Catalytic Active Site”
V. Habibpour, C. Yin, G. Kwon, Z. Wang, S. Vajda and R. E. Palmer
J. Exp. Nanosci. **8**, 993-1003 (2013), DOI: 10.1080/17458080.2013.849821, [link](#)
- I-68.** “Oxidation and Reduction of Size-Selected Subnanometer Pd Clusters on Al₂O₃ Surface”
B. H. Mao, R. Chang, S. Lee, S. Axnanda, E. Crumlin, S. D. Wang, S. Vajda, Z. Liu
J. Chem. Phys. **138**, 214304-1-7 (2013), DOI: 10.1063/1.4807488, [link](#)
- I-67.** „Size-Dependent Subnanometer Pd Cluster (Pd₄, Pd₆ and Pd₁₇) Water Oxidation Electrocatalysis“,
G. Kwon, E. C. Tyo, C. Yin, G. A. Ferguson, J. DeBartolo, S. Seifert, R. E. Winans, A. J. Kropf, C. J. Heard, R. L. Johnston, J. P. Greeley, L. A. Curtiss, M. J. Pellin, and S. Vajda
ACS Nano **7**, 5808-5817 (2013), DOI: 10.1021/nn400772s , [link](#)
- I-66.** “Atomic Layer Deposition of a Submonolayer Catalyst for the Enhanced Photoelectrochemical Performance of Water Oxidation with Hematite”
S.C. Riha, B. M. Klahr, E. C. Tyo, S. Seifert, S. Vajda, M. J. Pellin, T. W. Hamann, and A. B. F. Martinson,
ACS Nano **7**, 2396-2405 (2013), DOI: 10.1021/nn305639z, [link](#)
- I-65.** “Structure Sensitivity of Oxidative Dehydrogenation of Cyclohexane over FeO_x and Au/Fe₃O₄ Nanocrystals”
S. Goergen, C. Yin, M. Yang, B. Lee , S. Lee, C. Wang, P. Wu, M. B. Boucher, G. Kwon, S. Seifert , R. E. Winans, S. Vajda, and M. Flytzani-Stephanopoulos,
ACS Catal. **3**, 529-539 (2013), DOI: 10.1021/cs3007582 , [link](#)
- I-64.** “Controlling the Particle Size of ZrO₂ Nanoparticles in Hydrothermally Stable ZrO₂/MWCNT Composites”
C. Liu, S. Lee, Dong Su, B. Lee, S. Lee, R. E. Winans, C. Yin, S. Vajda, L. Pfefferle, G. L. Haller,
Langmuir **28**, 17159–17167 (2012), DOI: 10.1021/la303545y, [link](#)
- I-63.** “Stable Subnanometer Cobalt Oxide Clusters on Ultrananocrystalline Diamond and Alumina Supports: Oxidation State and the Origin of Sintering-Resistance”
G. A. Ferguson, C. Yin, G. Kwon, S. Lee, J. P. Greeley, P. Zapol, B. Lee, S. Seifert, R. E. Winans, and S. Vajda, and L. A. Curtiss
J. Phys. Chem. C **116**, 24027–24034 (2012), DOI: 10.1021/jp3041956, [link](#)

- I-62.** “Oxidative Dehydrogenation of Cyclohexane on Cobalt Oxide (Co₃O₄) Nanoparticles: The Effect of Particle Size on Activity and Selectivity”
E. C. Tyo, C. Yin, M. Di Vece, Q. Qian, S. Lee, B. Lee, S. Seifert, R. E. Winans, R. Si, B. Ricks, S. Goergen, M. Rutter, B. Zugic, M. Flytzani-Stephanopoulos, Z. Wang, R. E. Palmer, M. Neurock, and S. Vajda
ACS Catal. **2**, 2409–2423 (2012), DOI: 10.1021/cs300479a, *invited paper*, [link](#)
- I-61.** “Support-Dependent Performance of Size-Selected Subnanometer Cobalt Cluster-Based Catalysts in the Dehydrogenation of Cyclohexene”
S. Lee, M. Di Vece, B. Lee, S. Seifert, R. E. Winans and S. Vajda
Chem. Cat. Chem. **4**, 1632-1637 (2012), DOI: 10.1002/cctc.201200294, *invited paper*, [link](#)
- I-60.** “CO Oxidation by Subnanometer Ag_xAu_{3-x} Supported Clusters via DFT Simulations”
F. R. Negreiros, L. Sementa, G. Barcaro, S. Vajda, E. Aprà, and A. Fortunelli
ACS Catal. **2**, 1860–1864 (2012), DOI: 10.1021/cs300275v, [link](#)
- I-59.** “Exploring Computational Design of Size-Specific Subnanometer Clusters Catalysts”
G. A. Ferguson, F. Mehmood, R. Rankin, J. P. Greeley, S. Vajda, and L. A. Curtiss
Top. Catal. **55**, 353-365 (2012), DOI 10.1007/s11244-012-9804-4, [link](#)
- I-58.** “Oxidative Dehydrogenation of Cyclohexene on Size Selected Subnanometer Cobalt Clusters: Improved Catalytic Performance via Evolution of Cluster-Assembled Nanostructures”
S. Lee, M. Di Vece, B. Lee, S. Seifert, R. E. Winans and S. Vajda
Phys. Chem. Chem. Phys., **14**, 9336 - 9342 (2012), DOI: 10.1039/c2cp40162b, *invited paper*, [link](#)
- I-57.** “A First-Principle Theoretical Approach to Heterogeneous Nanocatalysis”
F. R. Negreiros, E. Aprà, G. Barcaro, L. Sementa, S. Vajda, and A. Fortunelli
Nanoscale **4**, 1208-1219 (2012), DOI: 10.1039/c1nr11051a, [link](#)
- I-56.** “Simultaneous Measurement of X-ray Small Angle Scattering, Absorption, and Reactivity: A Continuous Flow Catalysis Reactor”
S. Lee, B. Lee, S. Seifert, S. Vajda and R. E. Winans
Nucl. Instr. and Meth. A, **649**, 200-203 (2011), DOI:10.1016/j.nima.2010.12.172, [link](#)
- I-55.** Communication: “Suppression of Sintering of Size-Selected Pd Clusters under Realistic Reaction Conditions for Catalysis”
F. Yin, S. Lee, A. Abdela, S. Vajda, and R. E. Palmer
J. Chem. Phys. **134**, 141101-1-4 (2011), DOI:10.1063/1.3575195, [link](#)
- I-54.** “Cleavage of the C-O-C bond on Size-Selected Subnanometer Cobalt Catalysts and on ALD-Cobalt Coated Nanoporous Membranes”
W. Deng, S. Lee, J. A. Libera, J. W. Elam, S. Vajda, and C. L. Marshall
Appl. Catal. A: General **393**, 29-35 (2011), DOI:10.1016/j.apcata.2010.11.022, [link](#)

- I-53.** “Size-Dependent Selectivity and Activity of Silver Nanoclusters in the Partial Oxidation of Propylene to Propylene Oxide and Acrolein: A Joint Experimental and Theoretical Study”
L. M. Molina, S. Lee, K. Sell, G. Barcaro, A. Fortunelli, B. Lee, S. Seifert, R. E. Winans, J. W. Elam, M. J. Pellin, I. Barke, A. Kleibert, V. von Oeynhausen, Y. Lei, R. J. Meyer, J. A. Alonso, A. Fraile-Rodríguez, S. Giorgio, C. R. Henry, K.-H. Meiwes-Broer and S. Vajda
Catal. Today **160**, 116-130 (2011), DOI:10.1016/j.cattod.2010.08.022, invited article, [link](#)
- I-52.** “Oxidative Decomposition of Methanol on Subnanometer Palladium Clusters: The Effect of Catalyst Size and Support Composition”
S. Lee, B. Lee, F. Mehmood, S. Seifert, J. A. Libera, J. W. Elam, J. Greeley, P. Zapol, L. A. Curtiss, M. J. Pellin, P. C. Stair, R. E. Winans, and S. Vajda
J. Phys. Chem. C **114**, 10342–10348 (2010), DOI: 10.1021/jp912220w, [link](#)
- I-51.** “Combined TPRx, *in situ* GISAXS and GIXAS Studies of Model Semiconductor-Supported Platinum Catalysts in the Hydrogenation of Ethene”
S. A. Wyrzgol, S. Schäfer, S. Lee, B. Lee, M. Di Vece, X. Li, S. Seifert, R. E. Winans, M. Stutzmann, J. A. Lercher, S. Vajda
Phys. Chem. Chem. Phys. **12**, 5585–5595 (2010), DOI: 10.1039/b926493k, *invited feature article*, [link](#)
2011 Editor’s Choice: Catalysis and surface chemistry - [link](#)
- I-50.** “Increased Silver Activity for Direct Propylene Epoxidation via Subnanometer Size Effects”
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- IV-1.** “Anomalous Grazing Incidence Small-Angle X-Ray Scattering Studies of Platinum Nanoparticles Formed by Cluster Deposition”
B. Lee, S. Seifert, S.J. Riley, G.Y. Tikhonov, N. A. Tomczyk, S. Vajda, R.E. Winans,
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V. Publications in books of abstracts - extended reviewed abstracts

- V-3.** “Strongly Size-Dependent Catalytic Activity and Selectivity of Monodisperse Gold and Silver Nanocatalysts in the Direct Oxidation of Propylene to Propylene Oxide”
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Extended reviewed abstract number OA57, Book of Abstracts, 14th International Congress on Catalysis, 2008
- V-2.** “Theoretical and Experimental Studies of Propane Dehydrogenation on Sub-nanometer Pt Clusters: Unique Activity and Selectivity to Propylene”
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- V-1.** “*In-situ*, Real-Time GISAXS and TPR Studies on Size Selected Cluster Catalyst: Understanding Size/Shape Effect in Catalysis “
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