

**List of Publications**  
**Eckhard Spohr**  
**Theoretical Chemistry**  
**University Duisburg-Essen**

17. Februar 2011

**2011**

- [103] **"Modeling Proton Transfer to Charged Silver Electrodes"**  
F. Wilhelm, W. Schmickler, R. Nazmutdinov, and E. Spohr *Electrochim. Acta*, submitted
- [102] **"Hydrogen Bonding in Narrow Protonated Polymer Electrolyte Pores"**  
M. A. Ilhan and E. Spohr *J. Electroanal. Chem.*, accepted
- [101] **"Ab initio Molecular Dynamics of Proton Networks in Narrow Polymer Electrolyte Pores"**  
M. A. Ilhan and E. Spohr *J. Phys.: Cond. Matt.*, in press
- [100] **"Oxygen adsorption at  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3(001)$  surfaces: Predictions from first principles"**  
S. Piskunov, T. Jacob, and E. Spohr, *Phys. Rev. B* 83, 073402, (2011)

**2010**

- [99] **"Proton transfer to charged platinum electrodes. A molecular dynamics trajectory study"**  
F. Wilhelm, W. Schmickler, and E. Spohr, *J. Phys.: Condens. Matter* 22, 175001, (2010)

**2009**

- [98] **"Far IR spectra of  $\text{Ag}_2\text{CdI}_4$  at temperature range 10-420 K: complementary experimental and first-principle theoretical study"**  
I. Karbovnyk, S. Piskunov, I. Bolesta, S. Belluci, M. Cestelli Guidi, M. Piccinini, E. Spohr, and A. I. Popov, *European Phys. J. B* 70, 443, (2009)
- [97] **"Electrostatic control of occupancy and valence selectivity in a charged nanometer-sized cylindrical pore"**  
E. Spohr, E. Sovyak, A. Trokhymchuk, and D. D. Busath, *Mat.-wiss u. Werkstofftechn.* 40, 247, (2009)
- [96] **"Proton Transport in Polymer Electrolyte Membranes using Theory and Classical Molecular Dynamics"**

A. A. Kornyshev and E. Spohr, in *Device and Materials Modeling in PEM Fuel Cells*, edited by S. J. Paddison and K. Promislow, pp. 349-363, Springer, Berlin / Heidelberg (2009)

## 2008

[95] "Electronic structure and thermodynamic stability of  $\text{LaMnO}_3$  and  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  (001) surfaces: Ab initio calculations"

S. Piskunov, E. Heifets, T. Jacob, E. Kotomin, D. E. Ellis, and E. Spohr, *Phys. Rev. B* 78, 121406, (2008)

[94] "A Model for Proton Transfer to Metal Electrodes"

F. Wilhelm, W. Schmickler, R. R. Nazmutdinov, and E. Spohr, *J. Phys. Chem. C* 112, 10814, (2008)

[93] "Proton-Conducting Polymer Electrolyte Membranes: Water and Structure in Charge"

M. Eikerling, A. A. Kornyshev, and E. Spohr, in *Fuel Cells*, edited by G. Scherer, Advances in Polymer Science, pp. 15-54, Springer, Berlin, Heidelberg (2008)

## 2007

[92] "Proton Generation and Transport in the Fuel Cell Environment: Atomistic Computer Simulations"

E. Spohr, *J. Computer-Aided Mater. Des., Supplement 1* 14, 253, (2007)

[91] "Monte Carlo Simulations of a Simple Lattice Model of Polymer Electrolyte Membranes"

E. Spohr, *J. Mol. Liq.* 136, 288, (2007)

[90] "Electronic and magnetic structure of  $\text{La}_{0.875}\text{Sr}_{0.125}\text{MnO}_3$  calculated by means of hybrid density functional theory"

S. Piskunov, E. Spohr, T. Jacob, E. Kotomin, and D. E. Ellis, *Phys. Rev. B* 76, 012410, (2007)

[89] "Adsorption of formic acid on Pt(111) in the presence of water"

C. Hartnig, J. Grimminger, and E. Spohr, *J. Electroanal. Chem.* 607, 133, (2007)

[88] "The role of water in the initial steps of methanol oxidation on Pt(211)"

C. Hartnig, J. Grimminger, and E. Spohr, *Electrochim. Acta* 52, 2236, (2007)

## 2006

[87] "MD Simulations of Proton Transport along a Surface Decorated with Sulfonate Groups"

S. Dokmaïrsijan and E. Spohr, *J. Mol. Liq.* 129, 92, (2006)

[86] "Computer Simulation of Low Temperature Fuel Cells and their Components"

A. A. Kulikovskiy and E. Spohr, in *Proceedings of the NIC Symposium 2006*, edited by G. Münster, D. Wolf, and M. Kremer, NIC Series, vol. 32, pp. 269-277, John von Neumann Institute of Computing, Forschungszentrum Jülich, Jülich, Germany (2006)

## 2001-2005

[85] "The role of water in the initial steps of methanol oxidation on Pt(111)"

C. Hartnig and E. Spohr, *Chem. Phys.* 319, 185, (2005)

[84] "Aqueous Pore Structure and Proton Dynamics in Solvated Nafion Membranes"

- D. Seeliger, C. Hartnig, and E. Spohr, *Electrochim. Acta* 50, 4234, (2005)
- [83] "Proton Transport in Polymer Electrolyte Fuel Cell Membranes"  
E. Spohr, in *Ionic Soft Matter: Modern trends in theory and applications*, edited by D. Henderson et al., NATO Science Series, vol. 206, pp. 361-379, Springer, Dordrecht, The Netherlands (2005)
- [82] "Proton Transport in Proton Conductors for Fuel Cell Applications: Simulations, Elementary Reactions and Phenomenology"  
K. D. Kreuer, S. J. Paddison, E. Spohr, and M. Schuster, *Chem. Rev.* 104, 4637, (2004)
- [81] "Modeling of Proton Transfer in Polymer Electrolyte Membranes on Different Time and Length Scales"  
P. Commer, C. Hartnig, D. Seeliger, and E. Spohr, *Mol. Simulation* 30, 755, (2004)
- [80] "Molecular Dynamics Simulations of Proton Transfer in a Model Nafion Pore"  
E. Spohr, *Mol. Simulation* 30, 107, (2004)
- [79] "Some Recent Trends in Computer Simulations of Aqueous Double Layers"  
E. Spohr, *Electrochim. Acta* 49, 23, (2003)
- [78] "Proton Transport in Polymer Electrolyte Membranes. Theory and MD Simulations"  
P. Commer, C. Hartnig, and E. Spohr, in *Proceedings of the 2nd European Fuel Cell Forum*, edited by U. Bossel, pp. 49-58, Lucerne, Switzerland (2003)
- [77] "Computer Simulations of a Monolayer of Like-charged Particles Condensed on an Oppositely-charged Flat Area"  
E. Spohr, A. Trokhymchuk, E. Sovyak, D. Henderson, and D. T. Wasan, *Mol. Sim.* 29, 755, (2003)
- [76] "Kinetics of Proton Transport in Water"  
A. A. Kornyshev, A. M. Kuznetsov, E. Spohr, and J. Ulstrup, *J. Phys. Chem. B* 107, 3351, (2003)
- [75] "The nature of water content effect on the proton transport in polymer electrolyte membrane"  
P. Commer, A. G. Cherstvy, E. Spohr, and A. A. Kornyshev, *Fuel Cells* 2, 127, (2002)
- [74] "Solubility of KF in water by Molecular Dynamics using Kirkwood intergration method"  
M. Ferrario, G. Ciccotti, E. Spohr, T. Cartailier, and P. Turq, *J. Chem. Phys.* 117, 4947, (2002)
- [73] "Electrochemical Interfaces: At the Border line"  
A. A. Kornyshev, E. Spohr, and M. A. Vorotyntsev, in *Encyclopedia of Electrochemistry*, edited by A. Bard et al., vol. 1, pp. 33-132, Wiley-VCH, New York (2002)
- [72] "Enhancing Proton Mobility in Polymer Electrolyte Membranes: Lessons from Molecular Dynamics Simulations"  
E. Spohr, P. Commer, and A. A. Kornyshev, *J. Phys. Chem. B* 106, 10560, (2002)
- [71] "Molecular Dynamics simulations of water and ion dynamics in the electrochemical double layer"  
E. Spohr, *Solid State Ionics* 150, 1, (2002)
- [70] "Mechanism of Macroion-Macroion Clustering Induced by the Presence of Trivalent Counterions"  
E. Spohr, B. Hribar, and V. Vlachy, *J. Phys. Chem. B* 106, 2343, (2002)
- [69] "Molecular Dynamics simulations of the association of nonpolar spheres in water"  
E. Spohr and D. Henderson, *J. Colloid Interf. Sci.* 246, 316, (2002)

## 1996-2000

- [68] "Glass transition and layering effects in confined water: a computer simulation study"  
P. Gallo, M. Rovere, and E. Spohr, *J. Chem. Phys.* 113, 11324, (2000)
- [67] "Supercooled Confined Water and the Mode Coupling Crossover Temperature"

- P. Gallo, M. Rovere, and E. Spohr, *Phys. Rev. Lett.* *85*, 4317, (2000)
- [66] "Comparison of charged sheets and corrected 3D Ewald calculations of long-range forces in slab geometry electrolyte systems with solvent molecules"
- P. Crozier, R. L. Rowley, E. Spohr, and D. Henderson, *J. Chem. Phys.* *112*, 9253, (2000)
- [65] "Non-exponential kinetic behavior of confined water"
- P. Gallo, M. Rovere, M. A. Ricci, C. Hartnig, and E. Spohr, *Europhys. Lett.* *49*, 183, (2000)
- [64] "Modifications of the hydrogen bond network of liquid water in a cylindrical SiO<sub>2</sub>"
- C. Hartnig, W. Witschel, E. Spohr, P. Gallo, M. Ricci, and M. Rovere, *J. Mol. Liq.* *85*, 127, (2000)
- [63] "Water and Aqueous Solutions at Interfaces"
- E. Spohr, in *Computational Methods in Colloid and Interface Science*, edited by M. Borówko, Surfactant Science Series, vol. 89, pp. 347-386, Marcel Dekker, New York (2000)
- [62] "Evidence of Glassy Behaviour of Water Molecules in Confined States"
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- [61] "Water in porous glasses. A computer simulation study"
- E. Spohr, C. Hartnig, P. Gallo, and M. Rovere, *J. Mol. Liq.* *80*, 165, (1999)
- [60] "Structure of Water at the Water/Metal Interface. Molecular Dynamics Computer Simulations"
- M. L. Berkowitz, I.-C. Yeh, and E. Spohr, in *Interfacial Electrochemistry. Theory, Experiment, and Applications*, edited by A. Wieckowski, pp. 33-45, Marcel Dekker, New York (1999)
- [59] "Computer Simulations of Electrochemical Interfaces"
- E. Spohr, in *Advances in Electrochemical Science and Technology*, edited by R. C. Alkire and D. M. Kolb, vol. Vol 6, pp. 1-61, Wiley-VCH, Weinheim (1999)
- [58] "Molecular Simulation of the Electrochemical Double Layer"
- E. Spohr, *Electrochim. Acta* *44*, 1697, (1999)
- [57] "Orientational Correlations Near Interfaces. Computer Simulations of Water and Electrolyte Solutions in Confined Environments"
- A. Kohlmeyer, C. Hartnig, and E. Spohr, *J. Mol. Liq.* *78*, 233, (1998)
- [56] "Molecular Dynamics Study of Electrolyte-Filled Pores"
- C. Hartnig, W. Witschel, and E. Spohr, *Ber. Bunsenges. Phys. Chem.* *102*, 1689, (1998)
- [55] "Computer Simulations of Water and Electrolyte Solutions in Confined Environments"
- P. A. Bopp, A. Kohlmeyer, and E. Spohr, *Electrochim. Acta* *43*, 2911, (1998)
- [54] "Computer Simulation of the Structure of the Electrochemical Double Layer"
- E. Spohr, *J. Electroanal. Chem.* *450*, 327, (1998)
- [53] "Adsorption of Water Molecules in Slit Pores"
- E. Spohr, A. Trokhymchuk, and D. Henderson, *J. Electroanal. Chem.* *450*, 281, (1998)
- [52] "A Molecular Dynamics study of the structure and dynamics of water in cylindrical pores"
- C. Hartnig, W. Witschel, and E. Spohr, *J. Phys. Chem. B* *107*, 1241, (1998)
- [51] "Effect of Electrostatic Boundary Conditions and System Size on the Interfacial Properties of Water and Aqueous Solutions"
- E. Spohr, *J. Chem. Phys.* *107*, 6342, (1997)
- [50] "Long-range Structure in Bulk Water"
- A. Kohlmeyer, W. Witschel, and E. Spohr, *Z. Naturforsch.* *52a*, 432, (1997)
- [49] "Ab initio Study of Structural Properties of Stage-1 Alkali Graphite Intercalation Compounds"
- C. Hartwigsen, W. Witschel, and E. Spohr, *Ber. Bunsenges. Phys. Chem.* *101*, 859, (1997)
- [48] "Computer Simulation of Hydrated Ions near a Mercury Electrode"
- B. Eck and E. Spohr, *Electrochim. Acta* *42*, 2779, (1997)

[47] **"Computer Simulation of the Structure and Dynamics of Water Near Metal Surfaces"**

E. Spohr, in *Solid-Liquid Electrochemical Interfaces*, edited by G. Jerkiewicz, M. P. Soriaga, K. Uosaki, and A. Wieckowski, ACS Symposium Series, vol. 656, pp. 31-44, ACS, Washington (1997)

[46] **"Charge Density and Charge Transfer in Stage-1 Alkali Graphite Intercalation Compounds"**

C. Hartwigsen, W. Witschel, and E. Spohr, *Phys. Rev. B* 55, 4953, (1997)

[45] **"Molecular Dynamics Simulation Studies of the Density Profiles of CF1 Water between (9-3) Lennard-Jones Walls"**

E. Spohr, *J. Chem. Phys.* 106, 388, (1997)

[44] **"Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model"**

A. Kohlmeyer, W. Witschel, and E. Spohr, *Chem. Phys.* 213, 211, (1996)

[43] **"The Temperature Dependence of the Transfer of an Iodide Ion"**

O. Pecina, W. Schmickler, and E. Spohr, *J. Electroanal. Chem.* 405, 239, (1995)

[42] **"Structure and Dynamics of Water and Hydrated Ions near Platinum and Mercury Surfaces as Studied by MD Simulations"**

E. Spohr, G. Tóth, and K. Heinzinger, *Electrochim. Acta* 41, 2131, (1996)

## 1991-1995

[41] **"Statistical mechanical simulations on properties of liquid pyridine"**

K. Sagarik and E. Spohr, *Chem. Phys.* 199, 73, (1995)

[40] **"Density Profiles of a Water / Liquid Mercury Interface"**

J. Böcker, E. Spohr, and K. Heinzinger, *Z. Naturforsch.* 50a, 611, (1995)

[39] **"Computermmodellierung von Grenzflächen zwischen wäßrigen und metallischen Phasen"**

E. Spohr, in *Proceedings der "Zweiten Ulmer Elektrochemische Tage"*, edited by W. Schmickler, Universitätsverlag Ulm (1995)

[38] **"Ion Adsorption on Metal Surfaces. The Role of Water-Metal Interactions"**

E. Spohr, *J. Mol. Liquids* 64, 91, (1995)

[37] **"SCF calculations of the interaction of alkali and halide ions with the mercury surface"**

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[36] **"On the Mechanism of Electrochemical Ion Transfer Reactions"**

O. Pecina, W. Schmickler, and E. Spohr, *J. Electroanal. Chem.* 394, 29, (1995)

[35] **"Computer Modeling of Interfaces between aqueous and metallic phases"**

E. Spohr, *Acta Chem. Scand.* 49, 189, (1995)

[34] **"Molecular Dynamics Simulation Studies of the Mercury-Water Interface"**

J. Böcker, R. R. Nazmutdinov, E. Spohr, and K. Heinzinger, *Surf. Sci.* 335, 372, (1995)

[33] **"Partial charge transfer of the iodide ion near a water / metal interface"**

R. R. Nazmutdinov and E. Spohr, *J. Phys. Chem.* 98, 5956, (1994)

[32] **"A computer simulation study of iodide ion solvation in the vicinity of a liquid water/metal interface"**

E. Spohr, *Chem. Phys. Lett.* 207, 214, (1993)

[31] **"Modelling Water at Platinum Surfaces"**

G. Nagy, K. Heinzinger, and E. Spohr, *Faraday Discuss.* 94, 307, (1992)

[30] **"Thermodynamic Properties of the BJH Model of Water from Combining MD Simulation and Optimized Cluster Theory"**

A. D. Trokhymchuk, M. F. Holovko, E. Spohr, and K. Heinzinger, Ukrainian Academy of Sciences, Institute for Condensed Matter Physics (IPCM), Lviv, Ukraine (1992)

[29] **"Combination of Computer Simulation Methods and Optimized Cluster Theory in Determining Equilibrium Properties of Electrolyte Solutions. I. General Expressions and Application to Pure Water"**

A. D. Trokhymchuk, M. F. Holovko, E. Spohr, and K. Heinzinger, *Mol. Phys.* 77, 903, (1992)

[28] **"A Molecular Dynamics and X-Ray Diffraction Study of MgCl<sub>2</sub> in Methanol"**

Y. Tamura, E. Spohr, K. Heinzinger, G. Pálincas, and I. Bakó, *Ber. Bunsenges. Phys. Chem.* 96, 147, (1992)

[27] **"Computer Simulation Studies of IR Laser Excitation of Water on a Metal Surface"**

E. Spohr and M. Wolfsberg, *Surf. Sci. Lett.* 253, L395, (1991)

[26] **"A Molecular Dynamics Simulation of an Aqueous Beryllium Chloride Solution"**

M. M. Probst, E. Spohr, K. Heinzinger, and P. Bopp, *Molec. Simulation* 7, 43, (1991)

[25] **"Computer Simulation Studies of the Adsorption of Water on a Metal surface"**

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## 1986-1990

[24] **"Entropy and Degenerate Rearrangements"**

E. Spohr and M. Wolfsberg, *J. Phys. Chem.* 94, 6511, (1990)

[23] **"Molecular Dynamics Studies of Lanthanum Chloride Solutions"**

W. Meier, P. Bopp, M. M. Probst, E. Spohr, and J.-I. Lin, *J. Phys. Chem.* 94, 4672, (1990)

[22] **"Computer Simulation of the Water/Platinum Interface. Dynamical Results"**

E. Spohr, *Chem. Phys.* 141, 87, (1990)

[21] **"Isothermal-isobaric Molecular Dynamics Simulation of Polymorphic Phase Transitions in Alkali Halides"**

I. Ruff, A. Baranyai, E. Spohr, and K. Heinzinger, *J. Non-Crystalline Sol.* 117, 87, (1990)

[20] **"Vibrational and Rotational Excitation in Collisions of Diatomic Molecules with Rigid Surfaces"**

E. Spohr and M. Wolfsberg, *Chem. Phys. Lett.* 165, 221, (1990)

[19] **"Structural Properties of the Ion-Dipole Model of Electrolyte Solutions near Charged and Uncharged Hard Walls"**

S. N. Bliotskyj, M. F. Holovko, O. O. Pizio, and E. Spohr, Ukrainian Academy of Sciences, Institute for Theoretical Physics (ITP), Kiev, Ukraine (1989)

[18] **"On the Hydration of the Beryllium Ion"**

M. M. Probst, E. Spohr, and K. Heinzinger, *Chem. Phys. Lett.* 161, 405, (1989)

[17] **"Computer Simulations of Water / Metal Interfaces"**

K. Heinzinger and E. Spohr, *Electrochim. Acta* 34, 1849, (1989)

[16] **"Computer Simulations of Water / Platinum Interfaces"**

E. Spohr, *J. Phys. Chem.* 93, 6171, (1989)

[15] **"Isothermal-Isobaric Molecular Dynamics Simulation of Solid-Liquid and Solid-Solid Phase Transitions in Rubidium Bromide"**

I. Ruff, A. Baranyai, E. Spohr, and K. Heinzinger, *J. Chem. Phys.* 91, 3148, (1989)

[14] **"Structural and Dynamical Properties of an LiCl · 3H<sub>2</sub>O Solution"**

Y. Tamura, K. Tanaka, E. Spohr, and K. Heinzinger, *Z. Naturforsch.* 43a, 1103, (1988)

[13] **"A Molecular Dynamics Study on the Water / Metal Interfacial Potential"**

E. Spohr and K. Heinzinger, *Ber. Bunsenges. Phys. Chem.* 92, 1358, (1988)

[12] **"A Molecular Dynamics Study of an Aqueous SrCl<sub>2</sub> Solution"**

E. Spohr, G. Pálincas, K. Heinzinger, P. Bopp, and M. M. Probst, *J. Phys. Chem.* 92, 6754, (1988)

- [11] "Molecular Dynamics Study of a Lithium Ion in Ammonia"  
S. V. Hannongbua, T. Ishida, E. Spohr, and K. Heinzinger, *Z. Naturforsch.* 43a, 572, (1988)
- [10] "Computer simulations of Water and Aqueous Electrolyte Solutions at Interfaces"  
E. Spohr and K. Heinzinger, *Electrochim. Acta* 33, 1211, (1988)
- [9] "Molecular Polarity and the Structure of Liquid Methanol"  
G. Pálincas, Y. Tamura, E. Spohr, and K. Heinzinger, *Z. Naturforsch.* 43a, 43, (1988)
- [8] "Computer Simulations of Water Interactions Near Single Crystal Surfaces"  
E. Spohr and G. Pálincas, in *Interactions of Water in Ionic and Nonionic Hydrates*, edited by H. Kleeberg, pp. 221, Springer Verlag, Heidelberg (1987)
- [7] "A Study on Excited States Dipole Moments of 9,9'-Bianthryl"  
W. Baumann, E. Spohr, H. Bischof, and W. Liptay, *J. Luminescence* 37, 227, (1987)
- [6] "Molecular Dynamics Study of a KCL Aqueous Solution: Dynamical Results"  
M. Migliore, S. L. Fornili, E. Spohr, and K. Heinzinger, *Z. Naturforsch.* 42a, 227, (1987)
- [5] "A Molecular Dynamics Study of the Structure of an LiCl · 3H<sub>2</sub>O Solution"  
K. Tanaka, N. Ogita, Y. Tamura, I. Okada, H. Ohtaki, G. Pálincas, and E. Spohr, *Z. Naturforsch.* 42a, 29, (1987)
- [4] "Molecular Dynamics and X-Ray Diffraction Study of Aqueous Beryllium(II) Chloride Solutions"  
T. Yamaguchi, H. Ohtaki, E. Spohr, G. Pálincas, and K. Heinzinger, *Z. Naturforsch.* 41a, 1175, (1986)
- [3] "A Molecular Dynamics Study of the Structure of an Aqueous KCl Solution"  
M. Migliore, S. L. Fornili, E. Spohr, G. Pálincas, and K. Heinzinger, *Z. Naturforsch.* 41a, 826, (1986)
- [2] "A Molecular Dynamics Study of an Aqueous LiI Solution between Lennard-Jones Walls"  
E. Spohr and K. Heinzinger, *J. Chem. Phys.* 84, 2304, (1986)
- [1] "Molecular Dynamics Simulation of a Water / Metal Interface"  
E. Spohr and K. Heinzinger, *Chem. Phys. Lett.* 123, 218, (1986)