CURRICULUM VITAE

NAME: LUKAS VLCEK

PERSONAL DATA

Home address	254 N. Purdue Ave., Apt. 102, Oak Ridge, TN 37830
Business address	Oak Ridge National Laboratory, Chemical Sciences Division, 1 Bethel Valley Road, Oak Ridge TN, 37 831, USA
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EDUCATION

2004	Ph.D. in physical chemistry, Institute of Chemical Technology, Prague, Czech Republic
1998	M.S. (with honors) in physical chemistry, Masaryk University, Brno, Czech Republic

EMPLOYMENT

2/2010 – present	Research Scientist at the Oak Ridge National Laboratory, Chemical Sciences Division, Oak Ridge, TN, USA. Performing simulation and theoretical study with the goal to develop an atomistic description of geochemical systems.
11/2004 - 2/2010	Research Associate at Vanderbilt University, Department of Chemical Engineering, Nashville, TN, USA. Performed simulation study of mineral-water interfaces.
1/2004 – 11/2004	Research Associate at the Institute of Chemical Process Fundamentals, Acad. of Sci. of the Czech Rep. Performed theoretical and simulations study of fluid thermodynamics.
6/1996 – 8/1996	Intern at the Institute of Biophysics, Acad. of Sci. of the Czech Rep. Performed electrochemical study of DNA.

PROFESSIONAL MEMBERSHIP

The American Institute of Chemical Engineers (since 2005)

The American Chemical Society (since 2007)

The Geochemical Society (since 2011)

REVIEWER FOR PROFESSIONAL JOURNALS

6 peer-reviewed journals: Journal of Physical Chemistry, Fluid Phase Equilibria, Langmuir, Surface Science, Philosophical Magazine, and Physical Chemistry Chemical Physics.

PUBLICATIONS

33 original research papers + 3 book chapters. Cited by >400 peer-reviewed articles. The Hirsh index (h-index): 13. Work presented at more than 20 international conferences.

Research papers

1. Rother G., Vlcek L., Gruszkiewicz M., Chialvo A.A., Anovitz L.M., Banuelos J.L., Wallacher D., Grimm N., Cole D.R., *J. Phys. Chem. C*, (2014) accepted.
2. Vlcek L., Chialvo A.A., Simonson J.M.: Correspondence between cluster-ion and bulk thermodynamic properties: on the validity of the cluster-pair-based approximation, *J. Phys. Chem. A*, 117(14), 11328-11338 (2013).
3. Chialvo A.A., Vlcek L., Cummings P.T.: Surface corrugation effects on the water-graphene interfacial and confinement behavior, *J. Phys. Chem. C*, 117(45), 23875-23886 (2013).
4. Li S., Han K.S., Feng G., Hagaman E.W., Vlcek L., Cummings P.T.: Dynamic and structural properties of room-temperature ionic liquids near silica and carbon surfaces, *Langmuir*, 29(31), 9744-9749 (2013).
5. Wang H.W., Wesolowski D.J., Proffen T.E., Vlcek L., Wang W., Allard L.F., Kolesnikov A.I., Feygenson M., Anovitz L.M., Paul R.L.: Structure and stability of SnO2 nanocrystals and surface-bound water species, *J. Am. Chem. Soc.*, 135(18), 6885-6895 (2013).
6. Wesolowski D.J., Sofo J.O., Bandura A.V., Zhang Z., Mamontov E., Predota M., Kumar N., Kubicki J.D., Vlcek L., Machesky M., Fenter P.A., Cummings P.T., Anovitz A.M., Skelton A.A, Rosenqvist J.: The Rutile(110)-Water Interface: A comment on "Structure and Dynamics of Liquid Water on Rutile TiO_2(110)" by L.-M. Liu, C. Zhang, G. Thornton and A. Michaelides, Phys. Rev B, 85(16), 167401 (2012).
7. Chialvo A.A., Vlcek L., Cole D.R., Aqueous CO2 solutions at silica surfaces and within nanopore environments: Insights from isobaric-isothermal molecular dynamics, *J. Phys. Chem.* C, 116(26), 13904-13916 (2012).
8. Wu C., Skelton A., Chen M., Vlcek L., Cummings P.T.: Modeling the interaction between integrin-binding peptide (RGD) and rutile surface: the effect of cation mediation on Asp adsorption, *Langmuir*, 28(5), 2799-2811 (2012).
9. Wu C., Skelton A., Chen M., Vlcek L., Cummings P.T.: Modeling the interaction between integrin-binding peptide (RGD) and rutile surface: the effect of Na^+ on peptide adsorption, *J. Phys. Chem C*, 115(45), 22375-22386 (2011).
10. Vlcek L., Chialvo A.A, Cole D.R.: Optimized unlike-pair interactions for water-carbon dioxide mixtures described by the SPC/E and EPM2 models, *J. Phys. Chem B*, 115(27), 8775-8784 (2011).

11. Machesky M., Wesolowski D. J., Rosenqvist J., Predota M., Vlcek L., Ridley M., et al: Comparison of Cation Adsorption by Isostructural Rutile and Cassiterite, *Langmuir* 27(8), 4585-4593 (2011).
12. Cole D., Chialvo A.A., Rother G., Vlcek L., Cummings P.T.: Supercritical fluid behavior at nanoscale interfaces: Implications for CO2 sequestration in geologic formations, *Phil. Mag*. 90(17-18), 2339-2363 (2010).
13. Rosenqvist J., Machesky M.L., Vlcek L., Wesolowski, D.J.: Charging Properties of Cassiterite (α-SnO_2) surfaces in NaCl and RbCl ionic media, *Langmuir* 25 (18): 10852-10861 (2009).
14. Lajovic. A, Tomsic M., Fritz-Popovski G., Vlcek L., Jamnik A.: Exploring Structural Properties of Simple Aldehydes: Monte Carlo and Small-Angle X-Ray Scattering Study (Eng.) *Journal of Physical Chemistry B*, 113(28), 9429-9435 (2009).
15. Mamontov E., Vlcek L., Wesolowski D.J., Cummings P.T. et al.: Suppression of the dynamic transition in surface water at low hydration levels: A study of water on rutile (Eng.) *Phys. Rev. E.*.79, 051504 (2009).
16. Vlček L., Cummings P.T.: Adsorption of Water on TiO2 and SnO2 Surfaces: Molecular Dynamics Study. (Eng) Collect. Czech. Chem. Commun. 73(4), 575-589 (2008).
17. Machesky, M. et al: Surface Protonation at the Rutile (110) Interface: Explicit Incorporation of Solvation Structure within the Refined MUSIC Model Framework (Eng). Langmuir 24(21) 12331-12339 (2008).
18. Payne C.M., Zhao X., Vlček L., Cummings P.T.: Molecular dynamics simulations of ss-DNA translocation between copper nanoelectrodes incorporating electrode charge dynamics (Eng) J. Phys. Chem. B 112(6) 1712-1717 (2008).
19. Mamontov E., Wesolowski D.J., Vlček L.: Dynamics of Hydration Water on Rutile Studied by Backscattering Neutron Spectroscopy. (Eng) J. Phys. Chem. C, 112(32) 12334-12341 (2008).
20. Vlček L., Zhang Z., Machesky M.L., Fenter P., Rosenqvist J., Wesolowski D.J., Anovitz L.M., Předota M., Cummings P.T.: Electric Double Layer at Metal Oxide Surfaces: Static Properties of the Cassiterite-Water Interface. (Eng) Langmuir 23(9), 4925-4937 (2007).
21. Vlček L., Nezbeda I.: Excess Properties of Aqueous Mixtures of Methanol: Simple Models Versus Experiment. (Eng) J. Molec. Liquids 131/132, 158-162 (2007).
22. Tomšič M., Jamnik A., Vosecký V., Glatter O., Vlček L.: Structural Properties of Pure simple alcohols from ethanol, propanol, butanol, pentanol, to hexanol: Comparing Monte Carlo simulations with experimental SAXS data. (Eng) J. Phys. Chem. B 111(7), 1738-1751 (2007).
23. Tomšič M., Fritz-Popovski G., Vlček L., Jamnik A.: Calculating Small-Angle X-Ray Scattering Intensitiesfrom Monte Carlo Results: Exploring Different Approaches on the Example of Primary Alcohols. (Eng) Acta Chim. Slov. 54(3), 484-491 (2007).

24. Předota M., Vlček L.: Comment on Parts 1 and 2 of the Series “Electric Double Layer at the Rutile (110) Surface”. (Eng) J. Phys. Chem. B 111(5), 1245-1247 (2007).
25. Mamontov E., Vlček L., Wesolowski D.J., Cummings P.T., Wang W., Anovitz L.M., Rosenqvist J., Brown C.M., Garcia Sakai V.: Dynamics and Structure of Hydration Water on Rutile and Cassiterite Nanopowders Studied by Quasielastic Neutron Scattering and Molecular Dynamics Simulations. (Eng) J. Phys. Chem. C 111(11), 4328-4341 (2007).
26. Vlček L., Nezbeda I.: From Realistic to Simple Models of Fluids III. Primitive Models of Carbon Dioxide, Hydrogen Sulphide, and Acetone, and Their Properties. (Eng) Mol. Phys. 103(14), 1905-1915 (2005).
27. Vlček L., Nezbeda I.: Potential of Mean Force between Ions Infinitely Diluted Simple Short-Range Models of Aqueous Electrolytes. (Eng) Condensed Matter Phys. 8(2), 261-270 (2005).
28. Vlček L., Nezbeda I.: From Realistic to Simple Models of Associating Fluids. II. Primitive Models of Ammonia, Ethanol and Models of Water Revisited. (Eng) Mol. Phys. 102(5), 485-497 (2004).
29. Vlček L., Nezbeda I.: Thermodynamics of Simple Models of Associating Fluids: Primitive Models of Ammonia, Methanol, Ethanol, and Water. (Eng) Mol. Phys. 102(8), 771-781 (2004).
30. Nezbeda I., Vlček L.: Thermophysical Properties of Fluids: From Realistic to Simple Models and Their Applications. (Eng) Int. J. Thermophys. 25(4), 1037-1049 (2004).
31. Vlček L., Slovák J., Nezbeda I.: Thermodynamic Perturbation Theory of the Second-Order: Implementation for Models with Double-Bonded Sites. (Eng) Mol. Phys. 101(18), 2921-2927 (2003).
32. Vlček L., Nezbeda I.: From Realistic to Primitive Models: A Primitive Model of Methanol. (Eng) Mol. Phys. 101(19), 2987-2996 (2003).
33. Vlcek L., Nezbeda I.: Size and shape dependence of hydrophobic hydration at the level of primitive models, Phys. Chem. Chem. Phys 4(15), 3704-3711 (2002).

Book chapters

1. Chialvo A.A, Vlcek L., Cole D.R. ‘Acid Gases in CO2-rich Subsurface Geologic Environments’. In DePaolo D.J., et al. (eds.) ‘Geochemistry of Geologic CO2 Sequestration’, in Reviews in Mineralogy and Geochemistry, Vol 77, 361-398 (2013).
2. Vlcek L.; Ganesh P.; Bandura A.; Mamontov E.; Predota M.; Cummings P.T.; Wesolowski D.J. (2012) 'Modeling Interactions of Metal Oxide Surfaces with Water'. In: Korotcenkov G. (ed.) 'Chemical Sensors: Simulation and Modeling, Vol 1', Momentum Press, LLC.
3. Ross N.L., Spencer E.C., Levchenko A.A., Kolesnikov A.I., Wesolowski D.J., Cole D.R., Mamontov E., Vlcek L.: Studies of Mineral-Water Surfaces, in "Neutron Applications in Earth, Energy, and Environmental Sciences", Springer (2008).

OTHER SPECIAL SKILLS

Programming simulation software for parallel systems (C++, CUDA, Fortran, Python).
Advanced statistical data analysis (Bayesian methods).