

Luboš Vrbka - Publication list

- JOURNAL ARTICLES [16] Nachtigallová D., **Vrbka L.**, Bludský O., Nachtigall P., **Interaction of acetonitrile with Na-zeolites: Adsorption modes and vibrational dynamics in the zeolite channels and cavities**, *Phys. Chem. Chem. Phys.* **2008**, *10*, 4189–4198
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- [15] Bauerecker S., Ulbig P., Buch V., **Vrbka L.**, Jungwirth P., **Monitoring ice nucleation in pure and salty water via high speed imaging and computer simulations**, *J. Phys. Chem. C* **2008**, *112*, 7631–7636
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- [14] Otero Areán C., Rodríguez Delgado M., López Bauçà C., **Vrbka L.**, Nachtigall P., **Carbon monoxide adsorption on low-silica zeolites — from single to dual and to multiple cation sites**, *Phys. Chem. Chem. Phys.* **2007**, *9*, 4657–4661
doi:10.1039/b709073k
- [13] **Vrbka L.**, Jungwirth P., **Molecular dynamics simulations of freezing of water and salt solutions**, *J. Mol. Liq.* **2007**, *134*, 64–70
doi:10.1016/j.molliq.2006.12.011
- [12] Hrobárik T., **Vrbka L.**, Jungwirth P., **Selected biologically relevant ions at the air/water interface: A comparative molecular dynamics study**, *Biophys. Chem.* **2006**, *124*, 238–242
doi:10.1016/j.bpc.2006.04.010
- [11] **Vrbka L.**, Vondrášek J., Jagoda-Ćwiklik B., Vácha R., Jungwirth P., **Quantification and rationalization of the higher affinity of sodium over potassium to protein surface**, *Proc. Natl. Acad. Sci.* **2006**, *103*, 15440–15444
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- [10] **Vrbka L.**, Jungwirth P., **Homogeneous freezing of water starts in the subsurface**, *J. Phys. Chem. B* **2006**, *110*, 18126–18129
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- [9] **Vrbka L.**, Jungwirth P., Bauduin P., Touraud D., Kunz W., **Specific ion effects at protein surfaces: A molecular dynamics study of bovine pancreatic trypsin inhibitor and horseradish peroxidase in selected salt solutions**, *J. Phys. Chem. B* **2006**, *110*, 7036–7043
doi:10.1021/jp0567624
- [8] Petrov M., Minofar B., **Vrbka L.**, Jungwirth P., Kölsch P., Motschmann H., **Aqueous ionic and complementary zwitterionic soluble surfactants: Molecular dynamics simulations and sum frequency generation spectroscopy of the surfaces**, *Langmuir* **2006**, *22*, 2498–2505
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- [7] **Vrbka L.**, Jungwirth P., **Brine rejection from freezing salt solutions: A molecular dynamics study**, *Phys. Rev. Lett.* **2005**, *95*, 148501
doi:10.1103/PhysRevLett.95.148501
- [6] Winter B., Weber R., Hertel I. V., Faubel M., **Vrbka L.**, Jungwirth P., **Effect of bromide on the interfacial structure of aqueous tetrabutylammonium iodide: Photoelectron spectroscopy and molecular dynamics simulations**, *Chem. Phys. Lett.* **2005**, *410*, 222–227
doi:10.1016/j.cplett.2005.05.084
- [5] Minofar B., **Vrbka L.**, Mucha M., Jungwirth P., Yang X., Wang X.-B., Fu Y.-J., Wang L.-S., **Interior and interfacial aqueous solvation of benzene dicarboxylate dianions and their methylated analogues: A combined molecular dynamics and photoelectron**

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- [4] **Vrbka L.**, Jungwirth P., **Counter-ion effects and interfacial properties of aqueous tetrabutylammonium halide solutions**, *Austr. J. Chem.* **2004**, *57*, 1211–1217
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- [3] **Vrbka L.**, Mucha M., Minofar B., Jungwirth P., Brown E. C., **Propensity of soft ions for the air / water interface**, *Curr. Opin. Colloid Interface Sci.* **2004**, *9*, 67–73
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- [1] **Vrbka L.**, Klán P., Kříž Z., Koča J., Wagner P. J., **Computer modeling and simulations on flexible bifunctional systems: Intramolecular energy transfer implications**, *J. Phys. Chem. A* **2003**, *107*, 3404–3413
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PRESENTATIONS

- [5] **Vrbka L.**, Jungwirth P., **What can molecular simulations tell us about water freezing?**, *RHi international workshop on upper tropospheric humidity, June 11th–16th 2007*, Karlsruhe, Germany
- [4] **Vrbka L.**, Jungwirth P., **Ion solvation at surfaces of hydrated proteins and other interfaces: A molecular dynamics study**, *ESF exploratory workshop "Ch@ins: the limits of neutrality"*, **September 14th–15th 2006**, Compiègne, France
- [3] **Vrbka L.**, Jungwirth P., **Molecular simulations of water freezing: Brine rejection and homogeneous nucleation**, *Physics and Chemistry of Ice 2006, July 23rd–28th 2006*, Bremerhaven, Germany
- [2] **Vrbka L.**, Jungwirth P., **Biologically relevant ions at the air/water and protein/water interfaces**, *230th ACS National Meeting, August 2005*, Washington D.C., USA
- [1] **Vrbka L.**, Klán P., Kříž Z., Koča J., Wagner P. J., **Conformational behaviour of flexible molecules with two chromophores**, *XLV. Meeting of the Polish Chemical Society, September 2002*, Krakow, Poland

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- [1] **Vrbka L.**, Kunz W., **Theoretical description of ionic solutions using integral equation theory**, *Alexander von Humboldt Foundation Network Meeting, February 13th–15th 2008*, Marburg, Germany

BOOKS

- [1] **Vrbka L.**, Jungwirth P., **Molecular simulations of water freezing: Brine rejection and homogeneous nucleation**; in Kuhs W. F. (Ed.), *Physics and Chemistry of Ice, 2007*, Royal Society of Chemistry Publishing, ISBN (print) 978-0-85404-350-7, ISBN (online) 978-1-84755-777-3
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