# PCCP



**Physical Chemistry Chemical Physics** 

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## Water at interfaces

Guest Editor: Martin McCoustra

#### Editorial

<u>Water at interfaces</u> Phys. Chem. Chem. Phys., 2008, **10**, 4676 **DOI:** 10.1039/b812223g

Communications

#### Spectroscopic and computational evidence for SO<sub>2</sub> ionization on 128 K ice surface

B. Jagoda-Cwiklik, J. P. Devlin and V. Buch, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4678 **DOI:** <u>10.1039/b809839p</u>

## On the complete basis set limit and plane-wave methods in first-principles simulations of water

Susan B. Rempe, Thomas R. Mattsson and K. Leung, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4685 **DOI:** <u>10.1039/b810017a</u>

#### Papers

#### Lattice match in density functional calculations: ice lh vs. β-Agl

Peter J. Feibelman, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4688

DOI: 10.1039/b808482n

A proton between two waters: insight from fulldimensional quantum-dynamics simulations of the [H<sub>2</sub>O– H–OH<sub>2</sub>]<sup>±</sup> cluster Oriol Vendrell and Hans-Dieter Meyer, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4692 DOI: <u>10.1039/b807317a</u>

Molecular dynamics investigation of the intrinsic structure of water–fluid interfaces via the intrinsic sampling method Fernando Bresme, Enrique Chacón and Pedro Tarazona, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4704 **DOI:** 10.1039/b807437m

## An accurate analytic representation of the water pair potential

Wojciech Cencek, Krzysztof Szalewicz, Claude Leforestier, Rob van Harrevelt and Ad van der Avoird, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4716 **DOI:** <u>10.1039/b809435g</u>

#### Characterization of interfacial water in MOF-5

## (Zn<sub>4</sub>(O)(BDC)<sub>3</sub>)—a combined spectroscopic and theoretical study

K. Schröck, F. Schröder, M. Heyden, R. A. Fischer and M. Havenith, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4732 **DOI:** <u>10.1039/b807458p</u>

# Water confined in reverse micelles-probe tool in biomedical informatics

Florin Despa, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4740 **DOI:** <u>10.1039/b805699b</u>

#### Raman spectra of complexes of HNO<sub>3</sub> and NO<sub>3</sub> with NO<sub>2</sub> at surfaces and with N<sub>2</sub>O<sub>4</sub> in solution

Michael A. Kamboures, Wytze van der Veer, R. Benny Gerber and Leon F. Phillips, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4748

DOI: <u>10.1039/b810081k</u>

#### Molecular level structure of the liquid/liquid interface. Molecular dynamics simulation and ITIM analysis of the water-CCI<sub>4</sub> system

Lívia B. Pártay, George Horvai and Pál Jedlovszky, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4754 **DOI:** 10.1039/b807299j

#### Solvent structures of mixed water/acetonitrile mixtures at chromatographic interfaces from computer simulations

Jörg Braun, Antony Fouqueau, Raymond J. Bemish and Markus Meuwly, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4765 **DOI:** <u>10.1039/b807492e</u>

# Ion spatial distributions at the liquid-vapor interface of aqueous potassium fluoride solutions

Matthew A. Brown, Raffaella D<sup>\*</sup>Auria, I.-F. William Kuo, Maria J. Krisch, David E. Starr, Hendrik Bluhm, Douglas J. Tobias and John C. Hemminger, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4778

DOI: <u>10.1039/b807041e</u>

### Trapping proton transfer intermediates in the disordered hydrogen-bonded network of cryogenic hydrofluoric

#### acid solutions

Patrick Ayotte, Sylvain Plessis and Patrick Marchand, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4785 **DOI:** <u>10.1039/b806654j</u>

## Aqueous divalent metal-nitrate interactions: hydration versus ion pairing

Man Xu, James P. Larentzos, Mazen Roshdy, Louise J. Criscenti and Heather C. Allen, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4793 **DOI:** 10.1039/b807090n

# Structure and dynamics of water at a clay surface from molecular dynamics simulation

Virginie Marry, Benjamin Rotenberg and Pierre Turq, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4802 **DOI:** 10.1039/b807288d

#### Proton mobility in thin ice films: a revisit

Eui-Seong Moon, Chang-Woo Lee and Heon Kang, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4814 **DOI:** <u>10.1039/b807730b</u>

#### Thermodynamics of water intrusion in nanoporous hydrophobic solids

Fabien Cailliez, Mickael Trzpit, Michel Soulard, Isabelle Demachy, Anne Boutin, Joël Patarin and Alain H. Fuchs, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4817 **DOI:** <u>10.1039/b807471b</u>

#### Gas phase hydration of organic ions

Paul O. Momoh and M. Samy El-Shall, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4827 **DOI:** <u>10.1039/b809440n</u>

#### Water photodissociation in free ice nanoparticles at 243 nm and 193 nm

Viktoriya Poterya, Michal Fárník, Milan Ončák and Petr Slavíč ek, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4835 **DOI:** <u>10.1039/b806865h</u>

#### Electroacoustic and ultrasonic attenuation measurements of droplet size and *g*-potential of alkane-in-water emulsions: effects of oil solubility and composition

Alex M. Djerdjev and James K. Beattie, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4843 **DOI:** <u>10.1039/b807623e</u>

## Gas hydrate nucleation and cage formation at a water/methane interface

Robert W. Hawtin, David Quigley and P. Mark Rodger, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4853 **DOI:** <u>10.1039/b807455k</u>

#### <u>Hydration water rotational motion as a source of</u> <u>configurational entropy driving protein dynamics.</u> <u>Crossovers at 150 and 220 K</u>

J.-M. Zanotti, G. Gibrat and M.-C. Bellissent-Funel, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4865 **DOI:** 10.1039/b808217k

#### Influence of wettability and surface charge on the interaction between an aqueous electrolyte solution and a solid surface

Svetlana Guriyanova and Elmar Bonaccurso, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4871 **DOI:** 10.1039/b806236f

#### Molecular dynamics study of hydrated imogolite 2. Structure and dynamics of confined water

Benoît Creton, Daniel Bougeard, Konstantin S. Smirnov, Jean
Guilment and Olivier Poncelet, *Phys. Chem. Chem. Phys.*,
2008, **10**, 4879 **DOI:** 10.1039/b803479f

## Assessing the performance of implicit solvation models at a nucleic acid surface

Feng Dong, Jason A. Wagoner and Nathan A. Baker, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4889 **DOI:** <u>10.1039/b807384h</u>

#### Aqueous peptides as experimental models for hydration water dynamics near protein surfaces

Cecile Malardier-Jugroot, Margaret E. Johnson, Rajesh K. Murarka and Teresa Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4903 **DOI:** <u>10.1039/b806995f</u>

## Melting behavior of water in cylindrical pores: carbon nanotubes and silica glasses

M. Sliwinska-Bartkowiak, M. Jazdzewska, L. L. Huang and K. E. Gubbins, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4909 **DOI:** <u>10.1039/b808246d</u>

#### Increased interfacial thickness of the NaF, NaCl and NaBr salt aqueous solutions probed with non-resonant surface second harmonic generation (SHG)

Hong-tao Bian, Ran-ran Feng, Yan-yan Xu, Yuan Guo and Hong-fei Wang, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4920 **DOI:** <u>10.1039/b806362a</u>

#### Determination of the electron solvation site on D<sub>2</sub>O/Cu(111) using Xe overlayers and femtosecond photoelectron spectroscopy

Michael Meyer, Julia Stähler, Daniela O. Kusmierek, Martin Wolf and Uwe Bovensiepen, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4932

DOI: 10.1039/b807314g

## Breakdown of hydration repulsion between charged surfaces in aqueous Cs<sup>±</sup> solutions

Ronit Goldberg, Liraz Chai, Susan Perkin, Nir Kampf and Jacob Klein, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4939 **DOI:** <u>10.1039/b807459n</u>

#### A macroscopic water structure based model for describing charging phenomena at inert hydrophobic surfaces in aqueous electrolyte solutions

Johannes Lützenkirchen, Tajana Preočanin and Nikola Kallay, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4946 **DOI:** <u>10.1039/b807395c</u>

## Thermally induced mixing of water dominated interstellar ices

Daren J. Burke, Angela J. Wolff, John L. Edridge and Wendy A. Brown, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4956 **DOI:** <u>10.1039/b807220e</u>

## Water hydrogen bond analysis on hydrophilic and hydrophobic biomolecule sites

Daniela Russo, Jacques Ollivier and José Teixeira, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4968 **DOI:** <u>10.1039/b807551b</u>

#### Hydronium and hydroxide at the interface between water and hydrophobic media

Robert Vácha, Dominik Horinek, Max L. Berkowitz and Pavel Jungwirth, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4975 **DOI:** <u>10.1039/b806432f</u>

#### Average molecular orientations in the adsorbed water layers on silicon oxide in ambient conditions

Anna L. Barnette, David B. Asay and Seong H. Kim, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4981 **DOI:** <u>10.1039/b810309g</u>

Interfacial water structure at polymer gel/quartz interfaces investigated by sum frequency generation spectroscopy

Hidenori Noguchi, Minowa Hiroshi, Taiki Tominaga, Jian Ping Gong, Yoshihito Osada and Kohei Uosaki, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4987 **DOI:** <u>10.1039/b807297n</u>

#### Co-adsorption of water and hydrogen on Ni(111)

Junjun Shan, Jacques F. M. Aarts, Aart W. Kleyn and Ludo B. F. Juurlink, *Phys. Chem. Chem. Phys.*, 2008, **10**, 4994 **DOI:** <u>10.1039/b808219g</u>

#### Water-methanol mixtures: topology of hydrogen bonded network

Imre Bakó, Tünde Megyes, Szabolcs Bálint, Tamás Grósz and Viorel Chihaia, *Phys. Chem. Chem. Phys.*, 2008, **10**, 5004 **DOI:** <u>10.1039/b808326f</u>

## Characterization of interfacial water in MOF-5 $(Zn_4(O)(BDC)_3)$ a combined spectroscopic and theoretical study

K. Schröck,<sup>a</sup> F. Schröder,<sup>b</sup> M. Heyden,<sup>a</sup> R. A. Fischer<sup>b</sup> and M. Havenith<sup>a</sup>

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In this article we report the detection and characterization of adsorbed interfacial water within the cages of the metal–organic framework MOF-5  $(Zn_4O(BDC)_3)$  by terahertz time-domain spectroscopy (THz TDS) in the frequency range from 5 to 46 cm<sup>-1</sup>. The experimental spectra suggest a coupling of the intermolecular motions of the water molecules adsorbed to the collective vibrations of the network at 4 wt% hydration. This finding is supported by the results of MD simulations. When increasing the water content to 8 wt% we observed a non reversible decomposition of MOF-5.