

PCI 2006 Poster Presentation

Titel	Authors	Old No.	New No.
Ordering effects on bonding interactions in ice phases	Jenkins S. ¹ , Kirk S. ² , Ayers P. ³	P 001	002-P001
Structural and chemical character of ice X and higher pressure ice phases	Jenkins S. ¹ , Kirk S. ² , Ayers P. ³	P 002	005-P002
Real-space study of mechanical instability in ice XI on a "bond-by-bond" basis	Jenkins S. ¹ , Kirk S. ² , Ayers P. ³	P 003	008-P003
Structure, translational and orientational order of the amorphous ices	Saitta A.M. ¹ , Strässle T. ² , Klotz S. ³ , Saija F. ⁴ , Giaquinta P.V. ⁵	P 004	011-P004
Molecular mechanisms behind solid-liquid phase transition in ice micro-crystals. A molecular dynamics simulation study	Egorov A. ¹ , Brodskaya E. ² , Laaksonen A. ³	P 006	014-P005
Clusters which occur at interfaces of water and ice	Ziemczonek L. ¹	P 007	017-P006
Molecular dynamics simulations of organic compounds adsorbed on ice	Picaud S. ¹ , Hoang P.N.M. ¹	P 008	020-P007
Diffusion of formaldehyde and methanol in ice: A molecular dynamics study	Ballenegger V. ¹ , Picaud S. ¹ , Hoang P.N.M. ¹ , Toubin C. ²	P 009	028-P008
Structure of crystalline phases of Ice: static distortion and proton ordering	Kuo J.-L. ¹	P 010	031-P009
Solvation of nitrate ion and hydroxyl radical at the air/water and air/ice interface	Roeselová M. ¹ , Thomas J. ² , Dang L.X. ³ , Chang T.-M. ⁴ , Garrett B.C. ³ , Tobias D.J. ²	P 011	034-P010
Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice	Knight C. ¹ , Singer S.J. ¹	P 012	037-P011
Computer simulations of the 13 crystalline phase of ice	Baranyai A. ¹ , Bartok A. ¹ , Chialvo A. ²	P 013	040-P012
A combined micro-Raman and theoretical study of formaldehyde ice mixtures	Toubin C. ¹ , Chazallon B. ¹ , Focsa C. ¹	P 014	043-P013
HX photodissociation on ice : a quantum wave packets study	Woittequand S. ¹ , Briquez S. ¹ , Toubin C. ¹ , Monnerville M. ¹ , Pouilly B. ¹	P 015	046-P014
Theoretical study on gases in ice Ih investigated by the molecular orbital method	Hori A. ¹ , Hondoh T. ¹	P 016	049-P015
The bend angle of water in ice Ih: The significance of implementing the non-linear monomer Dipole Moment Surface in classical interaction potentials	Fanourgakis G. ¹ , Xantheas S. ¹	P 017	052-P 016
New approach for the pairwise potentials for water-water interactions	Aswani R. ¹ , Li J. ¹	P 018	055-P017
Percolating networks and liquid-liquid transitions in supercooled water	Oleinikova A. ¹ , Brovchenko I. ¹	P 019	003-P041
Isothermal amorphous-amorphous-amorphous transitions in H ₂ O	Winkel K. ¹ , Schustereder W. ² , Kohl I. ¹ , Salzmann C.G. ³ , Mayer E. ¹ , Loerting T. ⁴	P 020	006-P042
Observation of the glass transition of low density amorphous ice (LDA) and glycerol by isobaric volume-temperature experiments	Elsaesser M. ¹ , Kohl I. ¹ , Mayer E. ¹ , Loerting T. ²	P 021	012-P043
The local structure of ice VII determined by neutron total scattering	Guthrie M. ¹ , Bull C. ¹ , Nemes R. ¹ , Loveday J. ¹ , Strässle T. ² , Klotz S. ²	P 024	015-P044
Structural studies of the P-T behaviour of high density amorphous ices	Strässle T. ¹ , Bull C. ² , Guthrie M. ² , Loveday J. ² , Klotz S. ¹ , Nemes R. ²	P 025	018-P045
Hydrofluoric acid: a strong acid at low temperature	Ayotte P. ¹ , Marchand P. ¹ , Hébert M. ¹	P 026	021-P046
Raman scattering study of proton ordered ice-XI single crystal	Abe K. ¹ , Ootake Y. ¹ , Shigenari T. ¹	P 027	024-P047

Titel	Authors	Old No.	New No.
Extended low-frequency vibrations of hydrogen-bond networks of high and low density amorphous ices	Belosludov V.R. ¹ , Subbotin O.S. ¹ , Inerbaev T.M. ¹ , Belosludov R.V. ² , Kawazoe Y. ² , Rodger P.M. ³ , Shpakov V.P. ³ , Tse J.S. ⁴	P 028	030-P049
A new gibbs potential function for H2O ice Ih	Feistel R. ¹ , Wagner W. ²	P 029	033-P050
Phonon dispersion of ordinary ice up to 0.5 GPa: implications on the negative thermal expansion and pressure-induced amorphization of ice.	Strässle T. ¹ , Klotz S. ² , Saitta M. ² , Braden M. ³	P 030	036-P051
High pressure - high temperature studies on Ice VII and H2-H2O clathrate	Somayazulu M. ¹ , Goncharov A. ¹ , Mao H.-K. ¹ , Hemley R. ¹	P 031	039-P052
Mechanical strength and flow properties of ice-silicate mixture depending on the silicate contents and the silicate particle sizes	Yasui M. ¹ , Arakawa M. ²	P 032	042-P053
Effect of impurities on grain growth of ice	Azuma N. ¹ , Nishimura K. ¹ , Yokoyama S. ¹ , Takata M. ¹	P 033	045-P054
Methanol diffusion in ice	Marchand P. ¹ , Ayotte P. ¹	P 034	048-P055
Effects of freezing on aqueous mixtures of formaldehyde and ethanol investigated by micro-Raman spectroscopy	Chazallon B. ¹ , Toubin C. ¹ , Focsa C. ¹	P 035	053-P056
Grain boundary hierarchy in the EPICA-DML deep ice core, Antarctica	Hamann I. ¹ , Kipfstuhl S. ² , Faria S.H. ³ , Freitag J. ² , Lambrecht A. ⁴	P 036	056-P057
Freak patterns in the interface between polar ice and silicone oil	Kipfstuhl S. ¹ , Faria S.H. ² , Hamann I. ³ , Freitag J. ¹ , Wilhelms F. ¹	P 037	061-P058
Relaxation features in the EPICA ice cores	Kipfstuhl S. ¹ , Hamann I. ² , Faria S.H. ³ , Freitag J. ¹ , Wilhelms F. ¹	P 038	064-P059
Investigation of structural disorder in ice Ih using neutron diffraction and Reverse Monte Carlo modelling	Temleitner L. ¹ , Pusztai L. ¹	P 039	067-P060
Cryo-Atomic Force Microscopy (AFM) along Ice Surfaces	Krzyzak M. ¹ , Techmer K. ¹ , Genov G. ¹ , Kuhs W.F. ¹	P 040	001-P070
Experimental studies concerning photochemical reactions in snow	Jacobi H.-W. ¹ , Annor T. ¹ , Kwakye-Awuah B. ¹ , Hilker B. ¹ , Quansah E. ¹	P 041	004-P071
Molecular dynamics simulation of an ice nanocluster in supercooled water	Egorov A. ¹ , Brodskaya E. ²	P 042	007-P072
Comparison of a simple model of speedskate ice friction with measurements	Lozowski E. ¹ , Penny A. ¹	P 043	010-P073
AFM and SEM studies of frozen NaCl solutions	Krzyzak M. ¹ , Techmer K. ¹ , Kuhs W.F. ¹	P 044	013-P074
Grain boundary melting in polycrystalline ice	Thomson E. ¹ , Wettlaufer J. ¹ , Wilen L. ²	P 045	016-P075
Substrate effects on the interface melting of ice	Schoeder S. ¹ , Reichert H. ¹ , Engemann S. ¹ , Dosch H. ¹ , Bilgram J. ²	P 046	019-P076
Comparison of the specific surface area of natural and artificial snow samples measured using methane adsorption at 77 K and micro-tomography	Kerbrat M. ¹ , Huthwelker T. ¹ , Pinzer B. ² , Kaempfer T. ² , Schneebeli M. ² , Ammann M. ¹	P 047	022-P077
Surface melting of ice aAway from equilibrium	Cahoon A. ¹ , Wettlaufer J.S. ²	P 048	025-P078

Titel	Authors	Old No.	New No.
Dynamics of ice Ih films upon methanol adsorption: quasielastic neutron scattering experiments and molecular dynamics simulations	Picaud S. ¹ , Hoang P.N.M. ¹ , Lucas S. ² , Ferry D. ² , Demirdjian B. ² , Suzanne J. ²	P 049	026-P079
Ionisation of HCl on ice at very low temperature	Laffon C. ¹ , Parent P. ¹	P 050	032-P080
First-principles study of Bjerrum defects in ice Ih: An analysis of formation and migration properties.	de Koning M. ¹ , Antonelli A. ¹ , da Silva A.J.R. ² , Fazio A. ²	P 051	080-P063
First-principles study of molecular point defects in ice Ih: Interstitial vs. vacancy	de Koning M. ¹ , Antonelli A. ¹ , da Silva A.J.R. ² , Fazio A. ²	P 052	083-P064
First principles calculation of structure and dynamical properties of orientational defects in ice	Tsogbadrakh N. ¹ , Morrison I. ¹	P 053	088-P065
Dielectric relaxation of ice samples grown from water vapor or liquid	Takei I. ¹	P 055	091-P066
Microstructural deformation features in polar ice cores (EDML, Antarctica) and artificially deformed ice	Hamann I. ¹ , Kipfstuhl S. ² , Azuma N. ¹	P 056	094-P067
Formation of photoproducts and structural alterations in photon-irradiated crystalline and amorphous ices. A NEXAFS study.	Parent P. ¹ , Laffon C. ¹	P 057	099-P068
Optical study of heat generation and melting for gold NPs embedded into ice matrix	Richardson H. ¹ , Hickman Z. ¹ , Van Patten G. ¹ , Kordesch M. ² , Govorov A. ²	P 058	058-P018
Crystal orientations in quietly frozen ice sheets from fresh and brackish water	Müller-Stoffels M. ¹ , Langhorn P. ¹ , Petrich C. ¹ , Kempema E. ²	P 059	063-P019
Relationship between equilibrium and growth or melt shapes of disk crystals	Maruyama M. ¹	P 060	066-P020
Growth enhancement of ice crystal by impurity effect of AFGP or AFP molecules adsorbed on ice/water interface	Furukawa Y. ¹ , Terasawa T. ¹ , Nomura K. ¹ , Nishimura Y. ¹ , Zepeda S. ¹ , Yokoyama E. ²	P 061	070-P021
Water vapor transport in snow under temperature gradient condition	Kamata Y. ¹ , Sato A. ²	P 062	073-P022
Prediction of the cellular microstructure of sea ice by morphological stability theory	Maus S. ¹	P 063	076-P023
The planar-cellular transition during freezing of natural waters	Maus S. ¹	P 064	079-P024
Flow-induced morphological instability in sea ice	Neufeld J. ¹ , Wettlaufer J.S. ²	P 065	082-P025
Molecular-scale growth kinetics at ice-water interfaces: a molecular dynamics study using a new H2O potential model	Nada H. ¹ , Furukawa Y. ²	P 066	085-P026
FTIR study of the structure of antifreeze proteins at ice/water interfaces	Uda Y. ¹ , Kaneko F. ² , Matsuura Y. ³ , Zepeda S. ¹ , Furukawa Y. ¹	P 067	089-P027
Adsorption of antifreeze proteins on hydrophilic and hydrophobic surfaces	Zeng H. ¹ , Walker V. ² , Ripmeester J. ¹	P 068	092-P028
The growth of crystals and the transmission of light in frost surfaces	Smythe W. ¹ , Leu M.-T. ¹	P 069	097-P029
Crystal growth of ice I/hydrate eutectic binary solutions	McCarthy C. ¹ , Rieck K.D. ² , Kirby S.H. ³ , Durham W.B. ⁴ , Stern L.A. ³ , Cooper R.F. ¹	P 070	100-P030
The firnification of snow measured by X-Ray-micro-tomography at the EPICA-Drill site Dronning Maud Land (DML), Antarctica	Freitag J. ¹ , Kipfstuhl S. ¹ , Faria S.H. ²	P 071	103-P031
Nucleation of ice in SBA-silicas and carbon nanohorns	Dore J.C. ¹ , Webber J.B.W. ¹ , Seyed-Yazdi J. ¹ , Findenegg G.H. ² , Kaneko K. ³ , Tanaka H. ³	P 072	105-P032

Titel	Authors	Old No.	New No.
Possible use of Gaussian curvature for the 3D segmentation of snow grains from microtomographic data	Brzoska J.B. ¹ , Flin F. ² , Ogawa N. ³ , Lesaffre B. ¹	P 073	107-P033
Ripple formation mechanism on icicles under a thin shear flow	Ueno K. ¹ , Maeno N. ²	P 074	109-P034
Experimental evidence of liquid water formation during gas hydrate dissociation below the ice point	Melnikov V. ¹ , Nesterov A. ² , Reshetnikov A. ¹	P 075	041-P083
Microscopic model of structural phase transition in hydrates under pressure	Belosludov V.R. ¹ , Subbotin O.S. ¹ , Krupskii D.S. ¹ , Belosludov R.V. ² , Kawazoe Y. ²	P 076	044-P084
Effects of additives on formation rates of CO ₂ hydrate films	Uchida T. ¹ , Ikeda I.Y. ² , Ohmura R. ² , Tsuda S. ³	P 077	047-P085
High-pressure gas hydrates	Loveday J. ¹ , Maynard H. ¹ , Nelmes R. ¹ , Bull C. ¹ , Guthrie M. ¹	P 078	102-P069
Molecular dynamics simulations for structure-H hydrates of hydrocarbon large molecular guest substances	Miyoshi T. ¹ , Ohmura R. ² , Yasuoka K. ¹	P 079	050-P086
Classification of low-energy configurations of polyhedral water clusters from cube up to buckminsterfullerene	Kirov M. ¹	P 080	051-P087
Energy optimization of gas hydrate frameworks on the basis of discrete models of inter-molecular interactions	Kirov M. ¹	P 081	054-P088
Inelastic x-ray scattering studies on the vibrational dynamics of clathrate hydrates	Tse J. ¹ , Klug D. ² , Baumert J. ³ , Krisch M. ⁴	P 082	057-P089
Chemical and isotope gas composition of intrapermafrost shallow gas and gas-hydrate inclusions	Perlova E. ¹ , Makhonina N. ¹ , Leonov S. ¹ , Yakushev V. ¹	P 083	059-P090
Structure H hydrate kinetics studied by NMR spectroscopy	Susilo R. ¹ , Moudrakovski I.L. ² , Ripmeester J.A. ² , Englezos P. ¹	P 084	062-P091
Formation mechanisms of gas hydrate deposits in permafrost	Makhonina N. ¹ , Yakushev V. ¹	P 085	065-P092
Investigation of local pressure and network of hydrogen bonds in methane hydrate □ ice Ih system	Subbotin O.S. ¹ , Belosludov V.R. ¹ , Ikeshoji T. ² , Brodskaya E.N. ³ , Piotrovskaya E.M. ³ , Sizov V. ³	P 086	069-P093
Effects of large guest species on thermodynamic properties of structure-H hydrates	Makino T. ¹ , Sugahara T. ¹ , Ohgaki K. ¹	P 087	071-P094
Elastic properties of single-crystalline methane-ethylene hydrate under high pressure	Kato S. ¹ , Sasaki S. ¹ , Kume T. ¹ , Shimizu H. ¹	P 088	074-P095
Microscopic observation and in-situ Raman studies on some single-crystalline gas hydrates under high pressure	Sasaki S. ¹ , Kume T. ¹ , Shimizu H. ¹	P 089	077-P096
Formation of metastable gas hydrates structures and time dependency of their transformation into the stable crystalline form	Murshed M.M. ¹ , Klapproth A. ¹ , Seidel T. ¹ , Kuhs W.F. ¹	P 090	078-P097
High-resolution Raman spectra of N ₂ and O ₂ guest molecules in natural clathrate hydrates	Ohno H. ¹ , Hondoh T. ¹	P 091	081-P098
On the use of the Kihara potential for hydrate equilibrium calculations	Papadimitriou N. ¹ , Tsimpanogiannis I. ² , Yiotis A. ³ , Steriotis T. ³ , Stubos A. ³	P 092	084-P099
Formation of carbon dioxide gas hydrates in freezing sediments and decomposition kinetics	Chuvilin E. ¹ , Petrakova S. ¹ , Gureva O. ¹ , Istomin V. ²	P 093	086-P100
Investigation of methane hydrate dissociation through decay of radiation-induced methyl radical in methane hydrate	Takeya K. ¹ , Nango K. ¹ , Sugahara T. ¹ , Tani A. ² , Ohgaki K. ¹	P 094	090-P101

Titel	Authors	Old No.	New No.
Investigation of formation and phase diagrams of double gas hydrates H ₂ □ CH ₄ - H ₂ O at pressures up to 250 Mpa.	Skiba S. ¹ , Larionov E. ¹ , Manakov A. ¹	P 095	093-P102
Determination of volume changes upon phase transformations in the argon-water system	Ogienko A. ¹ , Tkacz M. ² , Manakov A. ¹ , Lipkowski J. ²	P 096	096-P103
Thermodynamic description of gas hydrate equilibria at high pressures	Istomin V. ¹ , Kwon V.G. ¹ , Durov V.A. ²	P 097	098-P104
Ordering mechanism of H ₂ O and gas molecules during growth of a gas clathrate hydrate	Nada H. ¹	P 098	101-P 105
From ice to CO ₂ hydrates and back □ The nature of formation and decomposition processes	Falenty A. ¹ , Genov G. ¹ , Kuhs W.F. ¹	P 099	104-P106
The hydrogen bonding nature of water molecules in methane hydrates as studied by in-situ low temperature IR spectroscopy	Ishikawa K. ¹ , Tani A. ¹ , Yoshida R. ¹	P 100	106-P107
Measurement of clathrate hydrates via infrared spectroscopy	Oyama H. ¹ , Jin Y. ¹ , Ebinuma T. ¹ , Nagao J. ¹ , Narita H. ¹	P 101	108-P108
Gas hydrates in sediments imaged by cryogenic SEM (CSEM): Insights from lab experiments on synthetic hydrates as interpretive guides	Kirby S. ¹ , Stern L. ²	P 102	110-P109
Microstructures of gas hydrates in porous media	Klapproth A. ¹ , Techmer K.S. ¹ , Klapp S.A. ¹ , Murshed M.M. ¹ , Kuhs W.F. ¹	P 103	111-P110
Special aspects of air hydrates in deep ice cores	Kipfstuhl S. ¹ , Hamann I. ² , Lambrecht A. ³ , Faria S.H. ⁴ , Freitag J. ¹ , Wilhelms F. ¹	P 105	113-P111
UV photolysis of amino acids in crystalline water ice: Can they survive on Europa?	Orzechowska G.E. ¹ , Goguen J.D. ¹ , Johnson P.V. ¹ , Kanik I. ¹	P 106	112-P035
Effects of additives and cooling rates on cryo-preservation process of rat cortical cells	Motomura J. ¹ , Uchida T. ¹ , Nagayama M. ¹ , Gohara K. ¹ , Taira T. ² , Shimizu K. ² , Sakai M. ²	P 107	114-P036
Fluorescence microscopy studies of ice surface - antifreeze proteins interactions	Pertaya N. ¹ , Marshall C.B. ² , DiPrinzio C.L. ¹ , Wilen L. ¹ , Thomson E. ³ , Wettlaufer J.S. ⁴ , Davies P.L. ² , Braslavsky I. ¹	P 109	116-P037
Anomalous dynamics of water in carbon nanotubes	Kolesnikov A.I. ¹ , Burnham C.J. ² , Loong C.-K. ¹ , de Souza N.R. ¹ , Reiter G. ² , Mamontov E. ³ , Mayers J. ⁴ , Adams M.A. ⁴ , Moravsky A.P. ⁵	P 111	118-P113
Chemistry induced by implantation of reactive ions in water ice	Strazzulla G. ¹ , Gomis O. ² , Leto G. ¹ , Spinella F. ¹	P 112	119-P039
Effect of snow accretion to the GPS antenna on positioning performance	Shishido M. ¹ , Yamamoto H. ² , Iikura S. ¹ , Endo T. ¹ , Masunari T. ³ , Okada K. ⁴ , Fujii T. ⁵	P 113	120-P114
Ice clusters in the size range of tens to thousands of water molecules	Buch V. ¹ , Baurecker S. ² , Devlin J.P. ³ , Buck U. ⁴ , C39 J. ⁵	P 114	122-P115
Air Permeability and Microstructure of Polar Firn at Hercules Dome, Antarctica	Hörhold M.W. ¹ , Albert M.R. ² , Freitag J. ¹	P 117	121-P 040

Titel	Authors	Old No.	New No.
Clathrate hydrate formation and growth: new experimental results versus modelled data	<u>Schicks J.1, Luzi M.1, Spangenberg E.2, Erzinger J.1</u>	-	023-P116
The growth and structure of ice XI	<u>Fukazawa H.¹, Igawa N.¹, Yamauchi H.¹, Ishii Y.¹, Hoshikawa A.¹, Chakoumakos B.C.², Fernandez-Baca J.A.²</u>	-	027-P048
Vibrational probe of the ice single crystal surface	<u>Shultz M.J.¹, Groenzin H.¹, Li I.¹</u>	-	035-P081
Water monolayers and ice films on Ru(0001) investigated with He atom scattering: Structure and stability under electron irradiation	<u>Traeger F.¹, Langenberg D.¹ and Wöll Ch.¹</u>	-	038-P082
High-density amorphous ice: Relaxation and crystallization between 0.2 and 1.9 GPa	<u>Salzmann C.G.¹, Loerting T.², Klotz S.³, Hallbrucker A.², Mayer E.²</u>	-	072-P061
Apparent Redistribution of Impurities and Air in the Near-Bedrock Ice of the EPICA DML Ice Core, Antarctica	<u>Kaufmann P.R.¹, Ruth U.², Kipfstuhl J.², Federer U.¹, Hutterli M.A.^{1,3}</u>	-	075-P062
Experimental and theoretical analysis of clathrate sII vibrations	<u>Militzer B.¹, Jenkins T.¹, Struzhkin V.¹, Mao W.², Mao H.K.¹, Hemley R.¹</u>	-	115-P112
Water adsorption on bio-membranes	<u>Günster J.¹, Souda R.²</u>	-	117-P038