# PUBLICATIONS

## OVERVIEW

49 papers (14 as first author, 5 as corresponding author) in peer reviewed journals, including
1 in *Reviews of Modern Physics*, 2 in Science, 3 in *PNAS*, 2 in *PRL* and 1 in *JACS* + 2 book chapter

# PEER-REVIEWED ARTICLES

[49] *Long range structures of amorphous solid water*
H. Li, A. Karina, M. Ladd-Parada, A. Späh, F. Perakis, C. Benmore, **K. Amann-Winkel#**
Journal of Physical Chemistry B 125 (48), 13320 (2021) # Corresponding author

[48] *Anomalous temperature dependence of the experimental x-ray structure factor of supercooled water*
N. Esmaeildoost, H. Pathak, A. Späh, T. J. Lane, K. H. Kim, C. Yang, **K. Amann-Winkel**, M. Ladd-Parada, F. Perakis, J. Koliyadu, A. R. Oggenfuss, P. JM Johnson, Y. Deng, S. Zerdane, R. Mankowsky, P. Beaud, H. T. Lemke, A. Nilsson, J. A. Sellberg
Journal of Chemical Physics 155 (21), 214501 (2021)

[47] *Enhancement and maximum in the isobaric specific-heat capacity measurements of deeply supercooled water using ultrafast calorimetry*
H. Pathak, A. Späh, N. Esmaeildoost, J. A. Sellberg, K. H. Kim, F. Perakis, **K. Amann-Winkel**, M. Ladd-Parada, J. Koliyadu, T. J. Lane, C. Yang, H. T. Lemke, A. R. Oggenfuss, P. J. M. Johnson, Y. Deng, S. Zerdane, R. Mankowsky, P. Beaud, A. Nilsson
Proceedings of the National Academy of Sciences U.S.A. (PNAS), 118, 6, (2021)

[46] *Experimental observation of the liquid-liquid transition in bulk supercooled water under pressure*
K. H. Kim*, **K. Amann-Winkel***, N. Giovambattista, A. Späh, F. Perakis, H. Pathak, M. Ladd Parada, C. Yang, D. Mariedahl, T. Eklund, T. J Lane, S. You, S. Jeong, M. Weston, J. Hyuk Lee, I. Eom, M. Kim, J. Park, S. H. Chun, P.H. Poole, A. Nilsson
*equally contributing to this work
SCIENCE 370, 6519, 978 (2020)

[45] *Electron beam induced transformation in high-density amorphous ices*
H. Xu, J. Ångström, T. Eklund, **K. Amann-Winkel#**
Journal of Physical Chemistry B 124 (41), 9283 (2020); # Corresponding author

[44] *Anisotropic X-Ray Scattering of Transiently Oriented water*
K. H. Kim, A. Späh, H. Pathak, C. Yang, S. Bonetti, **K. Amann-Winkel**, D. Mariedahl, D. Schlesinger, J. A. Sellberg, D. Mendez, G. van der Schot, H. Y. Hwang, J. Clark, O. Shigeki, T. Tadashi, Y. Harada, H. Ogasawara, T. Katayama, A. Nilsson, F. Perakis
Phys. Rev. Lett. 125, 076002 (2020)

[43] *Structural differences between unannealed and expanded high-density amorphous ice based on isotope substitution neutron diffraction*
**K. Amann-Winkel**, D. Bowron, T. Loerting
J. Mol. Phys. 117, 3207 (2019)

[42] *Temperature Dependent Anomalous Fluctuations in Water: Shift of 1 kbar Between Experiment and Classical Force Field Simulations*
H. Pathak, A. Späh, **K. Amann-Winkel**, F. Perakis, K. H. Kim and A. Nilsson
J. Mol. Phys. 117, 3232 (2019)

[41] *X-ray Studies of the Transformation from High-to Low-density Amorphous Water*
D. Mariedahl, F. Perakis, A. Späh, H. Pathak, K. Hwan Kim, C. Benmore, A. Nilsson, **K. Amann-Winkel#** # Corresponding author
Philos. Trans. Royal Soc. A, 377, 20180164 (2019)

[40] *Apparent Power-law behavior of water's isothermal compressibility and correlation length upon supercooling*
A. Späh, H. Pathak, K. H.Kim, F. Perakis, D.Mariedahl, **K. Amann-Winkel**, J. A. Sellberg, J. H. Lee, S.Kim, J. Park, K. H. Nam, T.Katayama, and A. Nilsson
Phys. Chem. Chem. Phys, 21, 26-31 (2019)

[39] *X-ray Scattering and O-O Pair-Distribution Functions of Amorphous Ices*
D. Mariedahl, F. Perakis, A. Späh, H. Pathak, K. H. Kim, G. Camisasca, D. Schlesinger, C. Benmore, L. G. M. Pettersson, A. Nilsson and **K. Amann-Winkel**[#]
[#] Corresponding author
Journal of Physical Chemistry B 122, 7616 (2018)

[38] *Response to comment on "Maxima in the Thermodynamic Response and Correlation Functions of Deeply Supercooled Water"*
K.H. Kim, A. Späh, H. Pathak, F. Perakis, D. Mariedahl, **K. Amann-Winkel**, J.A. Sellberg, J.H. Lee, S. Kim, J. Park, K.H. Nam, T. Katayama and A. Nilsson
SCIENCE 360, (2018)

[37] *Coherent x-rays reveal the influence of cage effects on ultrafast water dynamics*
F. Perakis, G. Camisasca, T. Lane, A. Späh, K. Wikfeldt, J. Sellberg, F. Lehmkühler, H. Pathak, K. H. Kim, **K. Amann-Winkel**, S. Schreck, S. Song, T. Sato, M. Sikorski, A. Eilert, T. McQueen, H. Ogasawara, D. Nordlund, W. Roseker, J. Koralek, S. Nelson, P. Hart, R. Alonso-Mori, Y. Feng, D. Zhu, A. Robert, G. Grübel, L. Pettersson, A. Nilsson
Nature Communications 9:1917 (*2018)*

[36] *Calorimetric study of water's two glass transitions in the presence of LiCl.*
G. N. Ruiz, **K. Amann-Winkel**, L. E. Bove, H. R. Corti, T. Loerting
Physical Chemistry Chemical Physics *20*, 6401 (2018)

[35] *Maxima in the Thermodynamic Response and Correlation Functions of Deeply Supercooled Water*
K.H. Kim, A. Späh, H. Pathak, F. Perakis, D. Mariedahl, **K. Amann-Winkel**, J.A. Sellberg, J.H. Lee, S. Kim, J. Park, K.H. Nam, T. Katayama and A. Nilsson
SCIENCE 358, 1589 (2017)

[34] *Relaxation dynamics and transformation kinetics of deeply supercooled water: Temperature, pressure, doping, and proton/deuteron isotope effects*
S. Lemke, P.H. Handle, L.J. Plaga, J.N. Stern, M. Seidl, V. Fuentes-Landete, **K. Amann-Winkel**, K.W. Köster, C. Gainaru, T. Loerting, and R. Böhmer
Journal of Chemical Physics 147, 034506, (2017)

[33] *Diffusive dynamics during the high-to-low density transition in amorphous ice*
F. Perakis[*], **K. Amann-Winkel**[*], F. Lehmkühler, M. Sprung, D. Mariedahl, J.A. Sellberg, H. Pathak, A. Späh, F. Cavalca, D. Schlesinger, A. Ricci, A. Jain, B. Massani, F. Aubree, C. J. Benmore, T. Loerting, G. Grübel, L. G. M. Pettersson and Anders Nilsson
[*]*equally contributing to this work*
Proceedings of the National Academy of Sciences U.S.A. (PNAS), 114, 8193, (2017)

[32] *X-ray and Neutron Scattering of Water*
**K. Amann-Winkel**, M.-C. Bellissent-Funel, L.E. Bove, T. Loerting, A. Nilsson, A. Paciaroni, D. Schlesinger, L. Skinner
Chemical Reviews 116, 13, 7570–7589, (2016)

[31] *Water: a Tale of Two Liquids.*
P. Gallo, **K. Amann-Winkel**, C.A. Angell, M. Anisimov, F. Chaupin, C. Chakravarty, E. Lascaris, T. Loerting, A. Panagiotopoulos, J. Russo, J.A. Sellberg, H. Stanley, H. Tanaka, C. Vega De Las Heras, L. Xu, L. Pettersson
Chemical Reviews 116, 13, 7463–7500, (2016)

[30] *Colloquium: water's controversial glass transitions*
**K. Amann-Winkel**, R. Böhmer, F. Fujara, C. Gainaru, B. Geil, T. Loerting
Reviews of Modern Physics *88*, 011002 (2016)

[29] *Experimental evidence for two distinct deeply supercooled liquid states of water. Response to „Comment on ‚Water's second glass transition'", by G. P. Johari,* Thermochim. Acta **617**, 200 *(2015)*
J. Stern, M. Seidl, C. Gainaru, V. Fuentes-Landete, **K. Amann-Winkel**, P. Handle, K.W. Köster, H. Nelson, R. Böhmer, T. Loerting
Thermochim. Acta (2015)

[28] *Anomalous behavior of the homogeneous ice nucleation rate in "no-man's land".*
H. Laksmono, T.A. McQueen, J.A. Sellberg, N. Duane Loh, C. Huang, D. Schlesinger, R.G. Sierra, C.Y. Hampton, D. Nordlund, M. Beye, A.V. Martin, A. Barty, M.M. Seibert, M. Messerschmidt, G.J. Williams, S. Boutet, **K. Amann-Winkel**, T. Loerting, L. G. M. Pettersson, M.J. Bogan, A. Nilsson
Journal of Physical Chemistry Letters 6, 2826 (2015)

[27] *The glass transition in high-density amorphous ice*
T. Loerting, V. Fuentes-Landete, P.H. Handle, M. Seidl, **K. Amann-Winkel**, C. Gainaru, R. Böhmer
Journal of Non-Crystalline Solids 407**,** 423 (2015)

[26] *Anomalously large isotope effect in the glass transition of water.*
C. Gainaru, A.L. Agapov, V. Fuentes-Landete, **K. Amann-Winkel**, H. Nelson, K.W. Köster, A.I. Kolesnikov, V.N. Novikov, R. Richert, R. Böhmer, T. Loerting, A.P. Sokolov
Proceedings of the National Academy of Sciences U.S.A. (PNAS) 111, 17402 (2014)

[25] *Water's second glass transition*
**K. Amann-Winkel**, C. Gainaru, P. H. Handle, M. Seidl, H. Nelson, R. Böhmer, T. Loerting
Proceedings of the National Academy of Sciences U.S.A. (PNAS) 110, 17720 (2013)

[24] *From parallel to single crystallization kinetics in high-density amorphous ice*
M. Seidl, **K. Amann-Winkel**, P. H. Handle, G. Zifferer, T. Loerting
Physical Review B 88, 174105 (2013)

[23] *Ultra-slow Dynamics in Low Density Amorphous Ice Revealed by Deuteron NMR: Indications for a Glass Transition*
F. Löw, **K. Amann-Winkel**, T. Loerting, F. Fujara, B. Geil
Physical Chemistry Chemical Physics 15, 9308 (2013)

[22] *Limits of metastability in amorphous ices: $^{2}$H-NMR relaxation*
F. Löw, **K. Amann-Winkel**, B. Geil, T. Loerting, *C. Wittich, F. Fujara*
Physical Chemistry Chemical Physics 15, 576 (2013)

[21] *Limits of metastability in amorphous ices: the neutron scattering Debye Waller factor*
**K. Amann-Winkel**, F. Löw, P.H. Handle, W. Knoll, J. Peters, B. Geil, F. Fujara, T. Loerting
Physical Chemistry Chemical Physics 14, 16386 (2012)

[20] *Local structural order in carbonic acid polymorphs: Raman and FT-IR spectroscopy*
C. Mitterdorfer, J. Bernard, F. Klauser, **K. Winkel**, I. Kohl, K.R. Liedl, H. Grothe, E. Mayer, T. Loerting
Journal of Raman Spectroscopy 43, 108 (2012)

[19] *Cryoflotation: densities of amorphous and crystalline ices*
T. Loerting, M. Bauer, I. Kohl, K. Watschinger, **K. Winkel**, E. Mayer
Journal of Physical Chemistry B 115, 14167 (2011)
Special Issue: H. Eugene Stanley Festschrift

[18] *How many amorphous ices are there?*
T. Loerting, **K. Winkel**, M. Seidl, M. Bauer, Ch. Mitterdorfer, P. H. Handle, Ch.G. Salzmann, E. Mayer, J.L. Finney, D. Bowron
Physical Chemistry Chemical Physics 13*, 8783 (2011)*

[17] *Equilibrated high-density amorphous ice and its first-order transition to the low-density form*
**K. Winkel**[#], E. Mayer, T. Loerting
[#] Corresponding authorship
Journal of Physical Chemistry B 115, 14141 (2011)
Special Issue: H. Eugene Stanley Festschrift

[16] *Volumetric study consistent with a glass-to-liquid transition in amorphous ices under pressure*
M. Seidl, M.S. Elsaesser, **K. Winkel**, G. Zifferer, E. Mayer, T. Loerting;
Physical Review B 83, 100201 (2011)

[15] *Structural study of low concentration LiCl aqueous solutions in the liquid, supercooled, and hyperquenched glassy states*
**K. Winkel**, M. Seidl, T. Loerting, L.E. Bove, S. Imberti, V. Molinero, F. Bruni,
R. Mancinelli, M.A. Ricci;
Journal of Chemical Physics 134, 024515 (2011)

[14] *Reversibility and isotope effect of the calorimetric glass→liquid transition of low-density amorphous ice*
M. S. Elsaesser, **K. Winkel**, E. Mayer, T. Loerting
Physical Chemistry Chemical Physics 12**,** 708 (2010)

[13] *Hexagonal ice transforms at high pressures and compression rates directly into "doubly metastable" ice phases*
M. Bauer, **K. Winkel**, D. Toebbens, E. Mayer, T. Loerting
Journal of Chemical Physics **131,** 224514 (2009)

[12] *Relaxation effects in low density amorphous ice:*
*Two distinct structural states observed by neutron diffraction*
**K. Winkel**, D.T. Bowron, T. Loerting, E. Mayer, J.L. Finney
Journal of Chemical Physics **130**, 204502 (2009)
**Research Highlight** at JCP online

[11] *Raman spectroscopic study of the phase transition of amorphous to crystalline ß-carbonic acid*
I. Kohl, **K. Winkel**, M. Bauer, K.R. Liedl, T. Loerting, E. Mayer
Angewandte Chemie Int. Ed. **48**, 2690 (2009)

[10] *Compression-rate dependence of the phase transition from hexagonal ice to ice II and/or ice III*
M. Bauer, M.S. Elsaesser, **K. Winkel**, E. Mayer, T. Loerting
Physical Review B **77**, 220105 (2008)

[9] *Structural transitions in amorphous $H_2O$ and $D_2O$: The effect of temperature*
**K. Winkel**, M. Bauer, E. Mayer, M. Seidl, M.S. Elsaesser, T. Loerting
Journal of Physics: Condensed Matter **20**, 494212 (2008)

[8] *Water polyamorphism: Reversibility and (dis)continuity*
**K. Winkel**, M.S. Elsaesser, E. Mayer, T. Loerting
Journal of Chemical Physics **128**, 044510 (2008)

[7] *Carbonic acid: From polyamorphism to polymorphism*
**K. Winkel**, W. Hage, T. Loerting, S.L. Price, E. Mayer
Journal of American Chemical Society **129**, 13863 (2007)

[6] *Isothermal amorphous- amorphous- amorphous transitions in water*
**K. Winkel**, W. Schustereder, I. Kohl, C.G. Salzmann, E. Mayer, T. Loerting
Proc. 11th Intl. Conf. on the Physics and Chemistry of Ice, 641 (2007)

[5] *High density amorphous ice from cubic ice*
T. Loerting, I. Kohl, W. Schustereder, **K. Winkel**, E. Mayer
Chem. Phys. Chem. **7**, 1203 (2006)

[4] *The relation between high-density and very-high-density amorphous ice*
T. Loerting, C.G. Salzmann, **K. Winkel**, E. Mayer
Physical Chemistry Chemical Physics **8**, 2810 (2006)

[3] *Amorphous ice: Stepwise formation of very-high-density amorphous ice from low-density amorphous ice at 125 K*
T. Loerting, W. Schustereder, **K. Winkel**, C.G. Salzmann, I. Kohl, E. Mayer
Physical Review Letters **96**, 025702 (2006)

[2] *Deuteron spin lattice relaxation in amorphous ices*
M. Scheuermann, B. Geil, **K. Winkel**, F. Fujara
Journal of Chemical Physics **124**, 224503 (2006)

[1] *Nature of amorphous polymorphism of water*
M.M. Koza, B. Geil, **K. Winkel**, C. Köhler, F. Czeschka, M. Scheuermann, H. Schober, T. Hansen; Physical Review Letters **94**, 125506 (2005)

## BOOK CHAPTER

*Crystalline and amorphous ices*
V. Fuentes-Landete, C. Mitterdorfer, P.H. Handle, G.N. Ruiz, J. Bernard, A. Bogdan, M. Seidl, **K. Amann-Winkel**, J. Stern, S. Fuhrmann, T. Loerting
In: P. G. Debenedetti, M. A. Ricci and F. Bruni (Eds.), *Proceedings of the International School of Physics "Enrico Fermi", Volume 187: Water: Fundamentals as the Basis for Understanding the Environment and Promoting Technology.* Amsterdam: IOS and Bologna: SIF 2015, 173–208.

*Amorphous ices*
Nicolas Giovambattista, **Katrin Amann-Winkel**, Thomas Loerting
*Advances in Chemical Physics, 152: Liquid Polymorphism;* John Wiley & Sons 2013, 139–173