

2025

309. M. Nolten, K.T. Xia, S. Pezzotti, G. Schwaab, R.G. Bergman, K.N. Raymond, F.D. Toste, T. Head-Gordon, W.L. Li, M. Havenith
Tuning the free energy of host-guest encapsulation by cosolvent
Phys. Chem. Chem. Phys., accepted (2025). DOI: 10.1039/d5cp00661a
308. S. Pezzotti, W. Chen, F. Novelli, X. Yu, C. Hoberg, M. Havenith
Terahertz-calorimetry spotlights the role of water in biological processes
Nat. Rev. Chem., accepted (2025). DOI: 10.1038/s41570-025-00712-8
307. A. Buchmann, L. Caminiti, L.L. Stiewe, S. Jung, D.M. Leitner, M. Havenith
Internal vibrational energy redistribution precedes energy dissipation into the solvent upon photoexcitation of heme proteins
Phys. Chem. Chem. Phys. **27**, 9470–9477 (2025). DOI: 10.1039/d5cp00797f
306. F. Novelli, A. Buchmann, I. Yousaf, L.L. Stiewe, W. Bronsch, F. Cilento, C. Hoberg, M. Havenith
High-mobility electrons in aqueous iodide solutions
ACS Omega **10**, 5097–5104 (2025). DOI: 10.1021/acsomega.4c11040
305. B. König, S. Pezzotti, G. Schwaab, M. Havenith
Tuning biological processes via co-solutes: from single proteins to protein condensates – the case of α -elastin condensation
Chem. Sci. **16**, 5897–5906 (2025). DOI: 10.1039/d4sc07335e
304. M. Havenith, M. Schnell, G. Niedner-Schatteburg
Spektroskopie und Quantenchemie: vom Mikrokosmos zur Anwendung
DPG-Publikation "Physik: Erkenntnisse und Perspektiven", 1. Auflage, 165–167 (2025).
ISBN 978-3-9826935-1-4
303. K. Mauelshagen, P. Schienbein, I. Kolling, G. Schwaab, D. Marx, M. Havenith
Random encounters dominate water-water interactions at supercritical conditions
Sci. Adv. **11**, eadp8614 (2025). DOI: 10.1126/sciadv.adp8614
302. R. Löscher, M.C. Schroeder, T. Vogel, A. Omar, A. Hasso, C. Hoberg, M. Havenith, C.J. Saraceno
Multi-milliwatt average power two-colour air-plasma terahertz source at 100 kHz repetition rate
Opt. Express **33**, 9213–9223 (2025). DOI: 10.1364/oe.546773
301. R.C. Cohen, K.R. Wilson, M. Havenith, L.M. Ziurys
A tribute to Richard J. Saykally
J. Phys. Chem. A **129**, 643–644 (2025). DOI: 10.1021/acs.jpca.4c08425
300. H. Ashraf, P. Meyer, S. Henkel, G. Schwaab, M. Havenith
IR spectra of the CH₃ stretching region of methylamine monomer, dimer and trimer in helium nanodroplets
Vib. Spectrosc. **136**, 103761 (2025). DOI: 10.1016/j.vibspec.2024.103761

2024

299. P. Meyer, S. Jäger, J. Khatri, S. Henkel, G. Schwaab, M. Havenith
Mixed H₂S and H₂O clusters – New insights into dispersion-dominated hydrogen bonding

- J. Phys. Chem. A **128**, 9627–9633 (2024). DOI: 10.1021/acs.jpca.4c05510
298. S. Jäger, J. Khatri, P. Meyer, S. Henkel, G. Schwaab, A. Nandi, P. Pandey, K.R. Barlow, M.A. Perkins, G.S. Tschumper, J.M. Bowman, A. van der Avoird, M. Havenith
On the nature of hydrogen bonding in the H₂S dimer
Nat. Commun. **15**, 9540 (2024). DOI: 10.1038/s41467-024-53444-6
297. S. Bag, R. Dec, S. Pezzotti, R.R. Sahoo, G. Schwaab, R. Winter, M. Havenith
Unraveling the hydration dynamics of the ACC₁₋₁₃K₂₄-ATP system: From liquid-to-droplet to-amyloid fibril
Biophys. J. **123**, 3863–3870 (2024). DOI: 10.1016/j.bpj.2024.09.011
296. S.S. Nalige, P. Galonska, P. Kelich, L. Sistemich, C. Herrmann, L. Vukovic, S. Kruss, M. Havenith
Fluorescence changes in carbon nanotube sensors correlate with THz absorption of hydration
Nat. Commun. **15**, 6770 (2024). DOI: 10.1038/s41467-024-50968-9
295. A. Chakraborty, S. Henkel, G. Schwaab, M. Havenith
Structural characterization of pyruvic acid dimer formed inside helium nanodroplets by infrared spectroscopy and ab initio study
J. Phys. Chem. A **128**, 5307–5313 (2024). DOI: 10.1021/acs.jpca.4c02203
294. B. König, S. Pezzotti, S. Ramos, G. Schwaab, M. Havenith
Real time measure of solvation free energy changes upon liquid-liquid phase separation of α -Elastin
Biophys. J. **123**, 1367–1375, (2024). DOI: 10.1016/j.bpj.2023.07.023
293. M. Koga, D.H. Kang, Z.N. Heim, P. Meyer, B.A. Erickson, N. Haldar, N. Baradaran, M. Havenith, D.M. Neumark
Extreme ultraviolet time-resolved photoelectron spectroscopy of adenine, adenosine and adenosine monophosphate in a liquid flat jet
Phys. Chem. Chem. Phys. **26**, 13106–13117 (2024). DOI: 10.1039/d4cp00856a
292. Y.H. Tao, S. Schulke, G. Schwaab, G.L. Nealon, S. Pezzotti, S.I. Hodgetts, A.R. Harvey, V.P. Wallace, M. Havenith
Hydration water drives the self-assembly of guanosine monophosphate
Biophys. J. **123**, 931–939 (2024). DOI: 10.1016/j.bpj.2024.03.005
291. D. Das Mahanta, D. Robinson Brown, T. Webber, S. Pezzotti, G. Schwaab, S. Han, M.S. Shell, M. Havenith
Bridging the gap in cryopreservation mechanism: Unraveling the interplay between structure, dynamics, and thermodynamics in cryoprotectant aqueous solutions
J. Phys. Chem. B **128**, 3720–3731 (2024). DOI: 10.1021/acs.jpcc.4c00264
290. S. Murke, W. Chen, S. Pezzotti, M. Havenith
Tuning acid-base chemistry at an electrified gold/water interface
J. Am. Chem. Soc. **146**, 12423–12430 (2024). DOI: 10.1021/jacs.3c13633
(Cover article – <https://pubs.acs.org/toc/jacsat/146/18>)
289. S. Mukherjee, S. Ramos, S. Pezzotti, A. Kalarikkal, T.M. Prass, L. Galazzo, D. Gendreizig, N. Barbosa, E. Bordignon, M. Havenith, L. Schäfer
Entropy tug-of-war determines solvent effects in the liquid-liquid phase separation of a globular protein
J. Phys. Chem. Lett. **15**, 4047–4055 (2024). DOI: 10.1021/acs.jpclett.3c03421

288. S. Schulke, M. Nolten, G. Schwaab, M. Havenith
Studying local electrostatics by terahertz spectroscopy using amines as a probe
ChemPhysChem **25**, e202300389 (2024). DOI: 10.1002/cphc.202300389
287. S. Pezzotti, A. Serva, C.J. Stein, M. Havenith
Adsorption of ions and solutes at electrified metal-aqueous interfaces: insights from THz spectroscopy and simulations
Encyclopedia of Solid-Liquid Interfaces, 66–80 (2024)
DOI: 10.1016/b978-0-323-85669-0.00092-1

2023

286. T. Ockelmann, C. Hoberg, A. Buchmann, F. Novelli, M. Havenith
Energy dissipation into the solvent during proton transfer occurs via acoustic phonons
J. Phys. Chem. B **127**, 9560–9565 (2023). DOI: 10.1021/acs.jpcc.3c04874
285. S. Bag, S. Pezzotti, D. Das Mahanta, S. Schulke, G. Schwaab, M. Havenith
From local hydration motifs in aqueous acetic acid solutions to macroscopic mixing thermodynamics: A quantitative connection from THz-calorimetry
J. Phys. Chem. B **127**, 9204–9210 (2023). DOI: 10.1021/acs.jpcc.3c06328
284. S. Ramos, J. Kamps, S. Pezzotti, K.F. Winklhofer, J. Tatzelt, M. Havenith
Hydration makes a difference! How to tune protein complexes between liquid–liquid and liquid–solid phase separation
Phys. Chem. Chem. Phys. **25**, 28063–28069 (2023). DOI: 10.1039/d3cp03299j
283. D. Das Mahanta, D.R. Brown, S. Pezzotti, S. Han, G. Schwaab, M.S. Shell, M. Havenith
Local solvation structures govern the mixing thermodynamics of glycerol–water solutions
Chem. Sci. **14**, 7381–7392 (2023). DOI: 10.1039/d3sc00517h
282. A.W. Hauser, M. Havenith, M. Koch, M. Sterrer
Festschrift for Wolfgang E. Ernst – electronic and nuclear dynamics and their interplay in molecules, clusters and on surfaces
Phys. Chem. Chem. Phys. **25**, 11880–11882 (2023). DOI: 10.1039/d3cp90052e
281. A. Leitenstorfer, ..., M. Havenith, ..., J. Cunningham
The 2023 terahertz science and technology roadmap
J. Phys. D: Appl. Phys. **56**, 223001 (2023). DOI: 10.1088/1361-6463/acbe4c
280. C. Hoberg, J.J. Talbot, J. Shee, T. Ockelmann, D. Das Mahanta, F. Novelli, M. Head-Gordon, M. Havenith
Caught in the act: real-time observation of the solvent response that promotes excited-state proton transfer in pyranine
Chem. Sci. **14**, 4048–4058 (2023). DOI: 10.1039/d2sc07126f
279. S. Pezzotti, B. König, S. Ramos, G. Schwaab, M. Havenith
Liquid–liquid phase separation? Ask the water!
J. Phys. Chem. Lett. **14**, 1556–1563 (2023). DOI: 10.1021/acs.jpclett.2c02697
278. F. Novelli, K. Chen, A. Buchmann, T. Ockelmann, C. Hoberg, T. Head-Gordon, M. Havenith
The birth and evolution of solvated electrons in the water
PNAS **120**, e2216480120 (2023). DOI: 10.1073/pnas.2216480120

277. H. Hao, E.M. Adams, S. Funke, G. Schwaab, M. Havenith, T. Head-Gordon
Highly altered state of proton transport in acid pools in charged reverse micelles
J. Am. Chem. Soc. **145**, 1826–1834 (2023). DOI: 10.1021/jacs.2c11331
276. S. Murke, K. Wonner, S. Alfarano, C. Rurainsky, P. Cignoni, K. Tschulik, M. Havenith
SERS reveals presence of Au-O-O-H and enhanced catalytic activity of electrochemically dealloyed AgAu nanoparticles
J. Phys. Chem. C **127**, 1071–1076 (2023). DOI: 10.1021/acs.jpcc.2c06515

2022

275. E.P. van Dam, B. König, S. Ramos, E.M. Adams, G. Schwaab, M. Havenith
Observation of dissipating solvated protons upon hydrogel formation
Phys. Chem. Chem. Phys. **24**, 27893–27899 (2022). DOI: 10.1039/d2cp01949c
274. S. Ruiz-Barragan, F. Sebastiani, P. Schienbein, J. Abraham, G. Schwaab, R. Raveendran, M. Havenith, D. Marx
Nanoconfinement effects on water in narrow graphene-based slit pores as revealed by THz spectroscopy
Phys. Chem. Chem. Phys. **24**, 24734–24747 (2022). DOI: 10.1039/d2cp02564g
273. S. Jäger, P. Meyer, K.-S. Feichtner, S. Henkel, G. Schwaab, V.H. Gessner, M. Havenith
Reaction of lithium hexamethyldisilazide (LiHMDS) with water at ultracold conditions
Phys. Chem. Chem. Phys. **24**, 24089–24094 (2022). DOI: 10.1039/d2cp03372k
272. D. Mani, T.K. Roy, J. Khatri, G. Schwaab, S. Blach, C. Hölzl, H. Forbert, D. Marx, M. Havenith
Internal electric field-induced formation of exotic linear-acetonitrile chains
J. Phys. Chem. Lett. **13**, 6852–6858 (2022). DOI: 10.1021/acs.jpclett.2c01482
271. F.N. Brüinig, M. Rammler, E.M. Adams, M. Havenith, R.R. Netz
Spectral signatures of excess-proton waiting and transfer-path dynamics in aqueous hydrochloric acid solutions
Nat. Commun. **13**, 4210 (2022). DOI: 10.1038/s41467-022-31700-x
270. S. Pezzotti, F. Sebastiani, E.P. van Dam, S. Ramos, V. Conti Nibali, G. Schwaab, M. Havenith
Spectroscopic fingerprints of cavity formation and solute insertion as a measure of hydration entropic loss and enthalpic gain
Angew. Chem. Int. Ed. **61**, e202203893 (2022). DOI: 10.1002/anie.202203893
Angew. Chem. **134**, e202203893 (2022). DOI: 10.1002/ange.202203893
269. G. Schwaab, R. Pérez de Tudela, D. Mani, N. Pal, T.K. Roy, F. Gabas, R. Conte, L. Durán Caballero, M. Ceotto, D. Marx, M. Havenith
Zwitter ionization of glycine at outer space conditions due to microhydration by six water molecules
Phys. Rev. Lett. **128**, 033001 (2022). DOI: 10.1103/PhysRevLett.128.033001
268. K. Wonner, S. Murke, S.R. Alfarano, P. Hosseini, M. Havenith, K. Tschulik
Operando electrochemical SERS monitors nanoparticle reactions by capping agent fingerprints
Nano Res. **15**, 4517–4524 (2022). DOI: 10.1007/s12274-021-3999-2
267. F. Novelli, C. Hoberg, E.M. Adams, J.M. Klopff, M. Havenith
Reply to the ‘Comment on “Terahertz pump–probe of liquid water at 12.3 THz”’ by A. F. G. van der Meer, PCCP, 2022, 24, D1CP05216K

Phys. Chem. Chem. Phys. **24**, 13413–13415 (2022). DOI: 10.1039/d2cp00565d

266. F. Novelli, C. Hoberg, E.M. Adams, J.M. Klopff, M. Havenith
Terahertz pump–probe of liquid water at 12.3 THz
Phys. Chem. Chem. Phys. **24**, 653–665 (2022). DOI: 10.1039/d1cp03207k
(Inside front cover: Phys. Chem. Chem. Phys. **24**, 598–598 (2022). DOI: 10.1039/d2cp90007f)

2021

265. A. Serva, M. Havenith, S. Pezzotti
The role of hydrophobic hydration in the free energy of chemical reactions at the gold/water interface: Size and position effects
J. Chem. Phys. **155**, 204706 (2021). DOI: 10.1063/5.0069498
264. T.K. Roy, K. Chatterjee, J. Khatri, G. Schwaab, M. Havenith
Helium nanodroplet infrared spectroscopy of oxazole-(water)_n (n = 1,2) clusters
AIP Adv. **11**, 115112 (2021). DOI: 10.1063/5.0066419
263. S.R. Alfarano, S. Pezzotti, C.J. Stein, Z. Lin, F. Sebastiani, S. Funke, C. Hoberg, I. Kolling, C.Y. Ma, K. Mauelshagen, T. Ockelmann, G. Schwaab, L. Fu, J.-B. Brubach, P. Roy, M. Head-Gordon, K. Tschulik, M.-P. Gaigeot, M. Havenith
Stripping away ion hydration shells in electrical double layer formation: Water networks matter
PNAS **118**, e2108568118 (2021). DOI: 10.1073/pnas.2108568118
262. T.K. Roy, D. Mani, G. Schwaab, M. Havenith
An infrared spectroscopic study of trifluoromethoxybenzene···methanol complexes formed in superfluid helium nanodroplets
Phys. Chem. Chem. Phys. **23**, 25180–25187 (2021). DOI: 10.1039/d1cp03136h
261. C.Y. Ma, S. Pezzotti, G. Schwaab, M. Gebala, D. Herschlag, M. Havenith
Cation enrichment in the ion atmosphere is promoted by local hydration of DNA
Phys. Chem. Chem. Phys. **23**, 23203–23213 (2021). DOI: 10.1039/d1cp01963e
260. E.M. Adams, H. Hao, I. Leven, M. Rüttermann, H. Wirtz, M. Havenith, T. Head-Gordon
Proton traffic jam: Effect of nanoconfinement and acid concentration on proton hopping mechanism
Angew. Chem. Int. Ed. **60**, 25419–25427 (2021). DOI: 10.1002/anie.202108766
Angew. Chem. **133**, 25623–25631 (2021). DOI: 10.1002/ange.202108766
259. J. Khatri, T.K. Roy, K. Chatterjee, G. Schwaab, M. Havenith
Vibrational spectroscopy of benzonitrile-(water)_{1–2} clusters in helium droplets
J. Phys. Chem. A **125**, 6954–6963 (2021). DOI: 10.1021/acs.jpca.1c04553
258. K. Chatterjee, T.K. Roy, J. Khatri, G. Schwaab, M. Havenith
Unravelling the microhydration frameworks of prototype PAH by infrared spectroscopy: Naphthalene-(water)_{1–3}
Phys. Chem. Chem. Phys. **23**, 14016–14026 (2021). DOI: 10.1039/d1cp01789f
257. K. Orend, C. Baer, F. Novelli, D. Welzel, T. Musch, M. Havenith
Designing a dielectric RF applicator cell for terahertz transmission
2021 ICEAA, IEEE, 177–182 (2021). DOI: 10.1109/ICEAA52647.2021.9539564
256. T.K. Roy, K. Chatterjee, J. Khatri, G. Schwaab, M. Havenith

- Stepwise microhydration of isoxazole: Infrared spectroscopy of isoxazole-(water)_n clusters in helium nanodroplets*
J. Phys. Chem. A **125**, 4766–4774 (2021). DOI: 10.1021/acs.jpca.1c01974
255. E. Adams, S. Pezzotti, J. Ahlers, M. Rüttermann, M. Levin, A. Goldenzweig, Y. Peleg, S. Fleischmann, I. Sagi, M. Havenith
Local mutations can serve as a game changer for global protein solvent interaction
JACS Au **1**, 1076–1085 (2021). DOI: 10.1021/jacsau.1c00155
254. I. Kolling, C. Hölzl, S. Imoto, S.R. Alfarano, H. Vondracek, L. Knake, F. Sebastiani, F. Novelli, C. Hoberg, J.-B. Brubach, P. Roy, H. Forbert, G. Schwaab, D. Marx, M. Havenith
Aqueous TMAO solution under high hydrostatic pressure
Phys. Chem. Chem. Phys. **23**, 11355–11365 (2021). DOI: 10.1039/d1cp00703c
253. S. Pezzotti, A. Serva, F. Sebastiani, F. Siro Brigiano, D.R. Galimberti, L. Potier, S. Alfarano, G. Schwaab, M. Havenith, M.-P. Gaigeot
Molecular fingerprints of hydrophobicity at aqueous interfaces from theory and vibrational spectroscopies
J. Phys. Chem. Lett. **12**, 3827–3836 (2021). DOI: 10.1021/acs.jpclett.1c00257
252. A. Serva, M. Salanne, M. Havenith, S. Pezzotti
Size-dependence of hydrophobic hydration at electrified gold/water interfaces
PNAS **118**, e2023867118 (2021). DOI: 10.1073/pnas.2023867118
251. J. Ahlers, E.M. Adams, V. Bader, S. Pezzotti, K.F. Winklhofer, J. Tatzelt, M. Havenith
The key role of solvent in condensation: mapping water in liquid-liquid phase-separated FUS
Biophys. J. **120**, 1266–1275 (2021). DOI: 10.1016/j.bpj.2021.01.019
250. F. Sebastiani, C.Y. Ma, S. Funke, A. Bäumer, D. Decka, C. Hoberg, A. Esser, H. Forbert, G. Schwaab, D. Marx, M. Havenith
Probing local electrostatics of glycine in aqueous solution by THz spectroscopy
Angew. Chem. Int. Ed. **60**, 3768–3772 (2021). DOI: 10.1002/anie.202014133
- 2016-2020**
249. F. Sebastiani, T.A. Bender, S. Pezzotti, W.-L. Li, G. Schwaab, R.G. Bergman, K.N. Raymond, F.D. Toste, T. Head-Gordon, M. Havenith
An isolated water droplet in the aqueous solution of a supramolecular tetrahedral cage
PNAS **117**, 32954–32961 (2020). DOI: 10.1073/pnas.2012545117
248. T.K. Roy, D. Mani, G. Schwaab, M. Havenith
A close competition between O-H...O and O-H... π hydrogen bonding: IR spectroscopy of anisole-methanol complex in helium nanodroplets
Phys. Chem. Chem. Phys. **22**, 22408–22416 (2020). DOI: 10.1039/d0cp02589e
247. F. Novelli, C.Y. Ma, N. Adhlakha, E.M. Adams, T. Ockelmann, D. Das Mahanta, P. Di Pietro, A. Perucchi, M. Havenith
Nonlinear terahertz transmission by liquid water at 1 THz
Appl. Sci. **10**, 5290 (2020). DOI: 10.3390/app10155290
246. V. Conti Nibali, S. Pezzotti, F. Sebastiani, D. Galimberti, G. Schwaab, M. Heyden, M.-P. Gaigeot, M. Havenith
Wrapping up hydrophobic hydration: Locality matters

- J. Phys. Chem. Lett. **11**, 4809–4816 (2020). DOI: 10.1021/acs.jpcllett.0c00846
245. F. Novelli, L. R. Pestana, K. C. Bennett, F. Sebastiani, E.M. Adams, N. Stavrias, T. Ockelmann, A. Colchero, C. Hoberg, G. Schwaab, T. Head-Gordon, M. Havenith
Strong anisotropy in liquid water upon librational excitation using terahertz laser fields
J. Phys. Chem. B **124**, 4989–5001 (2020). DOI: 10.1021/acs.jpcb.0c02448
244. F. Sebastiani, A.V. Verde, M. Heyden, G. Schwaab, M. Havenith
Cooperativity and ion pairing in magnesium sulfate aqueous solutions from the dilute regime to the solubility limit
Phys. Chem. Chem. Phys. **22**, 12140–12153 (2020). DOI: 10.1039/c9cp06845g
243. R. Schwan, C. Qu, D. Mani, N. Pal, G. Schwaab, J.M. Bowman, G.S. Tschumper, M. Havenith
Observation of the low frequency spectrum of water trimer as a sensitive test of the water trimer potential and the dipole moment surface
Angew. Chem. Int. Ed. **59**, 11399–11407 (2020). DOI: 10.1002/anie.202003851
(Frontispiece / Hot Paper: <https://onlinelibrary.wiley.com/doi/epdf/10.1002/anie.202082862>)
242. F. Novelli, B. Guchhait, M. Havenith
Towards intense THz spectroscopy on water: Characterization of optical rectification by GaP, OH1, and DSTMS at OPA wavelengths
MDPI Materials **13**, 1311 (2020). DOI: 10.3390/ma13061311
241. E. Adams, O. Lampret, B. König, T. Happe, M. Havenith
Solvent dynamics play a decisive role in the complex formation of biologically relevant redox proteins
Phys. Chem. Chem. Phys. **22**, 7451–7459 (2020). DOI: 10.1039/d0cp00267d
240. J. Deichmüller, F. Kogelheide, S. Murke, D. Hüther, G. Schwaab, P. Awakowicz, M. Havenith
Does plasma-induced methionine degradation provide alternative reaction paths for cell death?
J. Phys. D. **53**, 355401 (2020). DOI: 10.1088/1361-6463/ab8cea
239. S. Alfarano, H. Vondracek, F. Sebastiani, F. Novelli, C. Hoberg, I. Kolling, J.-B. Brubach, P. Roy, G. Schwaab, M. Havenith
Does hydrated glycine act as solidification nucleus at multi-kilobar conditions?
Biophys. Chem. **253**, 106215 (2019). DOI: 10.1016/j.bpc.2019.106215
238. D. Mani, R. Pérez de Tudela, R. Schwan, N. Pal, S. Körning, H. Forbert, B. Redlich, A.F.G. van der Meer, G. Schwaab, D. Marx, M. Havenith
Acid solvation versus dissociation at "stardust conditions": Reaction sequence matters
Sci. Adv. **5**, eaav8179 (2019). DOI: 10.1126/sciadv.aav8179
237. S. Funke, F. Sebastiani, G. Schwaab, M. Havenith
Spectroscopic fingerprints in the low frequency spectrum of ice (Ih), clathrate hydrates, supercooled water and hydrophobic hydration reveal similarities in the hydrogen bond network motifs
J. Chem. Phys. **150**, 224505 (2019). DOI: 10.1063/1.5097218
236. C. Hoberg, P. Balzerowski, M. Havenith
Integration of a rapid scanning technique into THz time-domain spectrometers for nonlinear THz spectroscopy measurements
AIP Adv. **9**, 035348 (2019). DOI: 10.1063/1.5080653

235. K. Lotz, A. Wütscher, H. Düdder, C. Berger, C. Russo, K. Mukherjee, G. Schwaab, M. Havenith, M. Muhler
Tuning the properties of iron-doped porous graphitic carbon synthesized by hydrothermal carbonization of cellulose and subsequent pyrolysis
ACS Omega **4**, 4448–4460 (2019). DOI: 10.1021/acsomega.8b03369
234. D. Mani, N. Pal, M. Smialkowski, C. Beakovic, G. Schwaab, M. Havenith
Accessing different binding sites of a multifunctional molecule: IR spectroscopy of propargyl alcohol...Water complexes in helium droplets
Phys. Chem. Chem. Phys. **21**, 20582–20587 (2019). DOI: 10.1039/c9cp02055a
(Inside front cover: Phys. Chem. Chem. Phys. **21**, 20504–20504 (2019). DOI: 10.1039/c9cp90233c)
233. R. Schwan, C. Qu, D. Mani, N. Pal, L. van der Meer, B. Redlich, C. Leforestier, J.M. Bowman, G. Schwaab, M. Havenith
Observation of the low frequency spectrum of water dimer as a sensitive test of the water dimer potential and dipole moment surfaces
Angew. Chem. Int. Ed. **58**, 13119–13126 (2019). DOI: 10.1002/anie.201906048
232. H. Vondracek, S. Alfarano, C.M. Hoberg, I. Kolling, F. Novelli, S. Sebastiani, J.-B. Brubach, P. Roy, G. Schwaab, M. Havenith
Urea's match in the hydrogen-bond network? A high pressure THz study
Biophys. Chem. **254**, 106240 (2019). DOI: 10.1016/j.bpc.2019.106240
231. G. Schwaab, F. Sebastiani, M. Havenith
Ion hydration and ion pairing as probed by THz spectroscopy
Angew. Chem. Int. Ed. **58**, 3000–3013 (2019). DOI: 10.1002/anie.201805261
230. G. Schwaab, F. Sebastiani, M. Havenith
Untersuchung von Ionenhydratation und Ionenpaarbildung mittels THz-Spektroskopie
Angew. Chem. **131**, 3030–3044 (2019). DOI: 10.1002/ange.201805261
229. H. Vondracek, S. Imoto, L. Knake, G. Schwaab, D. Marx, M. Havenith
Hydrogen-bonding in liquid water at multikilobar pressures
J. Phys. Chem. B **123**, 7748–7753 (2019). DOI: 10.1021/acs.jpcc.9b06821
228. F. Novelli, M. Bernal Lopez, G. Schwaab, B. Roldan Cuenya, M. Havenith
Water solvation of charged and neutral gold nanoparticles
J. Phys. Chem. B **123**, 6521–6528 (2019). DOI: 10.1021/acs.jpcc.9b02358
227. K. Mukherjee, G. Schwaab, M. Havenith
Cation-specific interactions of protein surface charges in dilute aqueous salt solutions: A combined study using dielectric relaxation spectroscopy and Raman spectroscopy
Phys. Chem. Chem. Phys. **20**, 29306–29313 (2018). DOI: 10.1039/c8cp05011b
226. H. Wirtz, S. Schäfer, C. Hoberg, K. Reid, D. Leitner, M. Havenith
Hydrophobic collapse of ubiquitin generates rapid protein-water motions
Biochemistry **57**, 3650–3657 (2018). DOI: 10.1021/acs.biochem.8b00235
225. A. Esser, H. Forbert, F. Sebastiani, G. Schwaab, M. Havenith, D. Marx
Hydrophilic solvation dominates the terahertz fingerprint of amino acids in water
J. Phys. Chem. B **122**, 1453–1459 (2018). DOI: 10.1021/acs.jpcc.7b08563
224. H. Wirtz, S. Schäfer, C. Hoberg, M. Havenith

- Differences in hydration structure around hydrophobic and hydrophilic model peptides probed by THz spectroscopy*
J. Infrared Millim. Terahertz Waves **39**, 816–827 (2018). DOI: 10.1007/s10762-018-0478-2
223. V. Conti Nibali, G. Morra, M. Havenith, G. D'Angelo, G. Colombo
Concerted motions on allosteric model proteins at terahertz frequencies
AAPP **96**, A6 (2018). DOI: 10.1478/AAPP.961A6
222. C. Klinkhammer, F. Böhm, V. Sharma, M. Seitz, G. Schwaab, M. Havenith
Anion dependent ion pairing in concentrated ytterbium halide solutions
J. Chem. Phys. **148**, 222802 (2018). DOI: 10.1063/1.5016549
221. M. Senske, Y. Xu, A. Bäumer, S. Schäfer, H. Wirtz, J. Savolainen, H. Weingärtner, M. Havenith
Local chemistry of the surfactant's head groups determines protein stability in reverse micelles
Phys. Chem. Chem. Phys. **20**, 8515–8522 (2018). DOI: 10.1039/c8cp00407b
220. D. Mani, T. Fischer, R. Schwan, A. Dey, B. Redlich, A.F.G. Van der Meer, G. Schwaab, M. Havenith
A helium nanodroplet setup for mid and far-infrared spectroscopy using pulsed-free-electron lasers: Vibrational spectra of propargyl alcohol
RSC Adv. **7**, 54318–54325 (2017). DOI: 10.1039/c7ra08102b
219. F. Sebastiani, S. Wolf, B. Born, T.Q. Luong, H. Cölfen, D. Gebauer, M. Havenith,
Water dynamics from THz spectroscopy reveals the locus of a liquid-liquid binodal limit in aqueous CaCO₃ solutions
Angew. Chem. Int. Ed. **56**, 490–495 (2017). DOI: 10.1002/anie.201610554
218. F. Sebastiani, S. Wolf, B. Born, T.Q. Luong, H. Cölfen, D. Gebauer, M. Havenith
THz-Spektroskopie erlaubt Rückschlüsse auf die Wasserdynamik und die Lage einer flüssig-flüssig-binodalen Grenze in wässrigen CaCO₃-Lösungen
Angew. Chem. **129**, 504–509 (2017). DOI: 10.1002/ange.201610554
217. V. Conti Nibali, G. Morra, M. Havenith, G. Colombo
Role of terahertz (THz) fluctuations in the allosteric properties of the PDZ domains
J. Phys. Chem. B **121**, 10200–10208 (2017). DOI: 10.1021/acs.jpcc.7b06590
216. K. Aoki, J. Savolainen, M. Havenith
Broadband terahertz pulse generation by optical rectification in GaP crystals
Appl. Phys. Lett. **110**, 201103 (2017). DOI: 10.1063/1.4983371
215. K. Sommer, M. Havenith
Lösungsmittel im Fokus der Forschung
Chem. Unserer Zeit **51**, 3 (2017). DOI: 10.1002/ciuz.201790003
214. M. Di Tucci, F. Böhm, G. Schwaab, E.R. Williams, M. Havenith
Effects of multivalent hexacyanoferrates and their ion pairs on water molecule dynamics measured with terahertz spectroscopy
Phys. Chem. Chem. Phys. **19**, 7297–7306 (2017). DOI: 10.1039/c6cp08423k
213. P. Schienbein, G. Schwaab, H. Forbert, M. Havenith, D. Marx
Correlations in the solute-solvent dynamics reach beyond the first hydration shell of ions
J. Phys. Chem. Lett. **8**, 2373–2380, (2017). DOI: 10.1021/acs.jpcclett.7b00713
212. E. Feresin, M. Havenith

- Solvatationsforschung ermittelt Rolle des Solvens: Das Lösungsmittel im Fokus*
Chem. Unserer Zeit **51**, 18–24 (2017). DOI: 10.1002/ciuz.201700781
211. D. Leicht, M. Kaufmann, N. Pal, G. Schwaab, M. Havenith
From the tunneling dimer to the onset of microsolvation: Infrared spectroscopy of allyl radical water aggregates in helium nanodroplets
J. Chem. Phys. **146**, 114306 (2017). DOI: 10.1063/1.4978482
210. F. Böhm, G. Schwaab, M. Havenith
Mapping hydration water around alcohol chains by THz calorimetry
Angew. Chem. Int. Ed. **56**, 9981–9985 (2017). DOI: 10.1002/anie.201612162
209. F. Böhm, G. Schwaab, M. Havenith
Kartierung des Hydratwassers um Alkoholketten mittels THz-Kalorimetrie
Angew. Chem. **129**, 10113–10117 (2017). DOI: 10.1002/ange.201612162
208. P.E. Decaneto, T. Vasilevskaya, Y. Kutin, H. Ogata, M. Grossman, I. Sagi, M. Havenith, W. Lubitz, W. Thiel, N. Cox
Solvent water interactions within the active site of the membrane type I matrix metalloproteinase
Phys. Chem. Chem. Phys. **19**, 30316–30331 (2017). DOI: 10.1039/c7cp05572b
207. C. Klinkhammer, C. Verlackt, D. Smilowicz, F. Kogelheide, A. Bogaerts, N. Metzler-Nolte, K. Stapelmann, M. Havenith, J. Lackmann
Elucidation of plasma-induced chemical modifications on glutathione and glutathione disulphide
Sci. Rep. **7**, 13828- (2017). DOI: 10.1038/s41598-017-13041-8
206. D. Gnutt, O. Brylski, E. Edengeiser, M. Havenith, S. Ebbinghaus
Imperfect crowding adaptation of mammalian cells towards osmotic stress and its modulation by osmolytes
Mol. BioSyst. **13**, 2218–2221 (2017). DOI: 10.1039/C7MB00432J
205. M. Engelhardt, K. Kartaschew, N. Bibino, M. Havenith, P. Awakowicz
Silicon surface modifications produced by non-equilibrium He, Ne, and Kr plasma jets
J. Phys. D **50**, 015206 (2017). DOI: 10.1088/1361-6463/50/1/015206
204. J.-W. Lackmann, M. Fiebrandt, M. Raguse, K. Kartaschew, M. Havenith, J. Bandow, R. Moeller, P. Awakowicz, K. Stapelmann
A combined low-pressure hydrogen peroxide evaporation plus hydrogen plasma treatment method for sterilization - Part 2: An intercomparison study of different biological systems
Plasma Process Polym. **14**, 1600199 (2017). DOI: 10.1002/ppap.201600199
203. A. Pougin, A. Lüken, C. Klinkhammer, D. Hiltrop, M. Kauer, K. Tölle, M. Havenith, K. Morgenstern, W. Grünert, M. Muhler, J. Strunk
Probing oxide reduction and phase transformations at the Au-TiO₂ interface by vibrational spectroscopy
Top. Catal. **60**, 1744–1753 (2017). DOI: 10.1007/s11244-017-0851-8
202. H. Jähme, G. Di Florio, V. Conti Nibali, C. Esen, A. Ostendorf, M. Grafen, E. Henke, J. Soetebier, C. Brenner, M. Havenith, M.R. Hofmann
Recognition of pharmaceuticals with compact mini-Raman-spectrometer and automatized pattern recognition algorithms

- Proceedings of SPIE **9899**, 98992M (2016). DOI: 10.1117/12.2228070
201. K. Kartaschew, S. Baldus, M. Mischo, E. Bründermann, P. Awakowicz, M. Havenith
Cold atmospheric-pressure plasma and bacteria: Understanding the mode of action using vibrational microspectroscopy
J. Phys. D. **49**, 374003 (2016). DOI: 10.1088/0022-3727/49/37/374003
200. M. Senske, D. Constantinescu-Aruxandei, M. Havenith, C. Herrmann, H. Weingärtner, S. Ebbinghaus
The temperature dependence of the Hofmeister series: Thermodynamic fingerprints of cosolute-protein interactions
Phys. Chem. Chem. Phys. **18**, 29698–29708 (2016). DOI: 10.1039/c6cp05080h
199. M. Engelhardt, R. Pothiraja, K. Kartaschew, N. Bibinov, M. Havenith, P. Awakowicz
Interaction of an argon plasma jet with a silicon wafer
J. Phys. D **49**, 145201 (2016). DOI: 10.1088/0022-3727/49/14/145201
198. D. Leicht, M. Kaufmann, R. Schwan, J. Schäfer, G. Schwaab, M. Havenith
Understanding the microsolvation of radicals: Infrared spectroscopy of benzyl radical water clusters
J. Chem. Phys. **145**, 204305 (2016). DOI: 10.1063/1.4968214
197. A. Bäumer, J. Duman, M. Havenith
Ice nucleation of an insect lipoprotein ice nucleator (LPIN) correlates with retardation of the hydrogen bond dynamics at the myo-inositol ring
Phys. Chem. Chem. Phys. **18**, 19318–19323 (2016). DOI: 10.1039/c6cp02399a
196. R. Schwan, M. Kaufmann, D. Leicht, G. Schwaab, M. Havenith
Infrared spectroscopy of the ν_2 band of the water monomer and small water clusters $(\text{H}_2\text{O})_{n=2,3,4}$ in helium droplets
Phys. Chem. Chem. Phys. **18**, 24063–24069 (2016). DOI: 10.1039/c6cp04333j
195. D. Leicht, M. Kaufmann, G. Schwaab, M. Havenith
Infrared spectroscopy of the helium solvated cyclopentadienyl radical in the CH stretch region
J. Chem. Phys. **145**, 074304 (2016). DOI: 10.1063/1.4960781
194. M.-C. Bellissent-Funel, A. Hassanali, M. Havenith, R. Henchman, P. Pohl, F. Sterpone, D. van der Spoel, Y. Xu, A.E. Garcia
Water determines the structure and dynamics of proteins
Chem. Rev. **116**, 7673–7697 (2016). DOI: 10.1021/acs.chemrev.5b00664
193. N. Samanta, T. Luong, D. Das Mahanta, R. Mitra, M. Havenith
Effect of short chain poly(ethylene glycol)s on the hydration structure and dynamics around human serum albumin
Langmuir **32**, 831–837 (2016). DOI: 10.1021/acs.langmuir.5b03884
192. P. Balzerowski, E. Bründermann, M. Havenith
Fabry-Pérot cavities for the terahertz spectral range based on high reflectivity multilayer mirrors
IEEE Trans. THz Sci. Technol. **6**, 563–567 (2016). DOI: 10.1109/TTHZ.2016.2572361
191. Y. Xu, A. Bäumer, K. Meister, C. Bischak, A. DeVries, D.M. Leitner, M. Havenith
Protein-water dynamics in antifreeze protein III activity
Chem. Phys. Lett. **647**, 1–6 (2016). DOI: 10.1016/j.cplett.2015.11.030

(Cover article / Frontiers article)

190. L. Knake, H. Vondracek, M. Havenith
A novel set-up to investigate the low-frequency spectra of aqueous solutions at high hydrostatic pressure
Rev. Sci. Instrum. **87**, 104101 (2016). DOI: 10.1063/1.4964099
189. T.Q. Luong, Y. Xu, E. Bründermann, D.M. Leitner, M. Havenith
Hydrophobic collapse induces changes in the collective protein and hydration low frequency modes
Chem. Phys. Lett. **651**, 1–7 (2016). DOI: 10.1016/j.cplett.2016.02.036
(Cover article / Frontiers article)
188. M. Kaufmann, D. Leicht, R. Schwan, D. Mani, G. Schwaab, M. Havenith
Helium droplet infrared spectroscopy of glycine and glycine-water aggregates
Phys. Chem. Chem. Phys. **18**, 28082–28090 (2016). DOI: 10.1039/c6cp05042e
187. M. Kaufmann, D. Leicht, M. Havenith, B.M Broderick, G.E. Douberly
Infrared spectroscopy of the tropyli radical in helium droplets
J. Phys. Chem. A **120**, 6768–6773 (2016). DOI: 10.1021/acs.jpca.6b06522
186. T. Fobbe, S. Markmann, F. Fobbe, N. Hekmat; H. Nong, S. Pal, P. Balzerowski, J. Savolainen, M. Havenith, A.D. Wieck, N. Jukam
Broadband terahertz dispersion control in hybrid waveguides
Opt. Express **24**, 22319–22333 (2016). DOI: 10.1364/oe.24.022319
185. F. Kogelheide, K. Kartaschew, M. Strack, S. Baldus, N. Metzler-Nolte, M. Havenith, P. Awakowicz, K. Stapelmann, J.-W. Lackmann
FTIR spectroscopy of cysteine as a ready-to-use method for the investigation of plasma-induced chemical modifications of macromolecules
J. Phys. D **49**, 084004 (2016). DOI: 10.1088/0022-3727/49/8/084004

2011-2015

184. E. Edengeiser, K. Meister, E. Bründermann, S. Büning, S. Ebbinghaus, M. Havenith
Non-invasive chemical assessment of living human spermatozoa
RSC Adv. **5**, 10424–10429 (2015). DOI: 10.1039/C4RA12158A
183. K. Kartaschew, M. Mischo, S. Baldus, E. Bründermann, P. Awakowicz, M. Havenith
Unraveling the interactions between cold atmospheric plasma and skin-components with vibrational microspectroscopy
Biointerphases **10**, 029516 (2015). DOI: 10.1116/1.4919610
182. R. Pothiraja, K. Kartaschew, N. Bibinov, M. Havenith, P. Awakowicz
Diamond single micro-crystals and graphitic micro-balls formation in plasmoids under atmospheric pressure
J. Phys. D **48**, 115201 (2015). DOI: 10.1088/0022-3727/48/11/115201
181. M. Havenith
Solvation Science: A new interdisciplinary field
Angew. Chem. Intl. Ed. **55**, 1218–1219 (2015). DOI: 10.1002/anie.201510614
180. D. Decka, G. Schwaab, M. Havenith

- A THz/FTIR fingerprint of the solvated proton: Evidence for Eigen structure and Zundel dynamics*
Phys. Chem. Chem. Phys. **17**, 11898–11907 (2015). DOI: 10.1039/C5CP01035G
179. F. Böhm, V. Sharma, G. Schwaab, M. Havenith
The low frequency modes of solvated ions and ion pairs in aqueous electrolyte solutions: iron(II) and iron(III) chloride
Phys. Chem. Chem. Phys. **17**, 19582–19591 (2015). DOI: 10.1039/C5CP03157E
178. L. Knake, G. Schwaab, K. Kartaschew, M. Havenith
Solvation dynamics of trimethylamine N-Oxide in aqueous solution probed by terahertz spectroscopy
J. Phys. Chem. B **119**, 13842–13851 (2015). DOI: 10.1021/acs.jpcc.5b04152
177. E. Decaneto, S. Suladze, Chr. Rosin, M. Havenith, W. Lubitz, R. Winter
Pressure and temperature effects on the activity and structure of the catalytic domain of human MT1-MMP
Biophys. J. **109**, 2371–2381 (2015). DOI: 10.1016/j.bpj.2015.10.023
176. S. Bauer, J. Stern, F. Böhm, C. Gainaru, M. Havenith, T. Loerting, R. Böhmer
Vibrational study of anharmonicity, supramolecular structure, and hydrogen bonding in two octanol isomers
Vib. Spectrosc. **79**, 59–65 (2015). DOI: 10.1016/j.vibspec.2015.05.001
175. D. Leicht, D. Habig, G. Schwaab, M. Havenith
Complexation of allyl radicals and hydrochloric acid in helium nanodroplets
J. Phys. Chem. A **119**, 1007–1012 (2015). DOI: 10.1021/jp511708s
174. Y. Xu, M. Havenith
Perspective: Watching low-frequency vibrations of water in biomolecular recognition by THz spectroscopy
J. Chem. Phys. **143**, 170901 (2015). DOI: 10.1063/1.4934504
173. D. Habig, D. Leicht, G. Schwaab, M. Havenith
Reassignment of $\nu_{2,3}$ IR band of the allyl radical in liquid helium nanodroplets
J. Chem. Phys. **143**, 024308 (2015). DOI: 10.1063/1.4923214
172. K. Hanke, M. Kaufmann, G. Schwaab, M. Havenith, C.T. Wolke, O. Gotlova, M.A. Johnson, B. Kar, W. Sander, E. Sánchez-García
Understanding the ionic liquid $[NC_{4111}][NTf_2]$ from individual building blocks: An IR-spectroscopic study
Phys. Chem. Chem. Phys. **17**, 8518–8529 (2015). DOI: 10.1039/c5cp00116a
171. D. Marx, K. Morgenstern, M. Havenith, M. Muhler
At the heart of the Ruhr metropolis: Bochum explores solvation science
Bunsen-Magazin **17**, 33–35 (2015).
170. K. Morgenstern, M. Havenith, D. Marx, M. Muhler
Solvation science – main topic of the Bunsentagung 2015
Bunsen-Magazin **17**, 36–37 (2015).
169. K. Morgenstern, D. Marx, M. Havenith, M. Muhler
Editorial of the PCCP themed issue on "Solvation Science"
Phys. Chem. Chem. Phys. **17**, 8295–8296 (2015). DOI: 10.1039/C5CP90022K

168. E. Edengeiser, J.-W. Lackmann, E. Bründermann, S. Schneider, J. Benedikt, J. E. Bandow, M. Havenith
Synergetic effects of atmospheric pressure plasma-emitted components on DNA oligomers: A Raman spectroscopic study
J. Biophotonics **8**, 918–924 (2015). DOI: 10.1002/jbio.201400123
167. H. Vondracek, J. Dielmann-Gessner, W. Lubitz, M. Knipp, M. Havenith
THz absorption spectroscopy of solvated β -lactoglobulin
J. Chem. Phys. **141**, 22D534 (2014). DOI: 10.1063/1.4903237
166. B. Born, M. Heyden, S. Ebbinghaus, M. Havenith
Probing solvation dynamics by terahertz absorption spectroscopy
In Terahertz biomedical science & technology, Editor J.-H. Son., CRC Press, 135–152 (2014).
165. J. Dielmann-Gessner, M. Grossman, V. Conti Nibali, B. Born, I. Solomonov, G.B. Fields, M. Havenith, I. Sagi
Enzymatic turnover of macromolecules generates long-lasting protein-water-coupled motions beyond reaction steady state
PNAS **111**, 17857–17862 (2014). DOI: 10.1073/pnas.1410144111
164. V. Sharma, F. Böhm, G. Schwaab, M. Havenith
The low frequency motions of solvated Mn(II) and Ni(II) ions and their halide complexes
Phys. Chem. Chem. Phys. **16**, 25101–25110 (2014). DOI: 10.1039/c4cp03989k
163. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith
Graphene multilayer as nano-sized optical strain gauge for polymer surface relief gratings
Nano Lett. **14**, 5754–5760 (2014). DOI: 10.1021/nl502631s
162. M. Heyden, G. Schwaab, M. Havenith,
Comment on "Hydration and mobility of trehalose in aqueous solution"
J. Phys. Chem. B. **118**, 10802–10805 (2014). DOI: 10.1021/jp508089t
161. M. Banerjee, V.-S. Dang; M. Bledowski, R. Radim; H.-W. Becker, D. Rogalla, E. Edengeiser, M. Havenith, A. Wieck, A. Devi,
MOCVD of TiO₂ thin films using a heteroleptic titanium complex: Precursor evaluation and investigation of optical, photoelectrochemical and electrical properties
Chem. Vap. Deposition **20**, 224–233 (2014). DOI: 10.1002/cvde.201407125
160. V. Conti Nibali, M. Havenith
New insights into the role of water in biological function: Studying solvated biomolecules using terahertz absorption spectroscopy in conjunction with molecular dynamics simulations
J. Am. Chem. Soc. **136**, 12800–12807 (2014). DOI: 10.1021/ja504441h
159. D. Habig, D. Leicht, M. Kaufmann, G. Schwaab, M. Havenith
IR-spectroscopic study of the allyl + NO reaction in helium nanodroplets
J. Chem. Phys. **141**, 044312 (2014). DOI: 10.1063/1.4890366
158. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith
Confocal Raman microscopy and AFM study of the interface between the photosensitive polymer layer and multilayer graphene
Soft Mater. **12**, 98–105 (2014). DOI: 10.1080/1539445X.2014.945040
157. A. Patra, T.Q. Luong, R.K. Mitra, M. Havenith

- The influence of charge on the structure and dynamics of water encapsulated in reverse micelles*
Phys. Chem. Chem. Phys. **16**, 12875–12883 (2014). DOI: 10.1039/c4cp00386a
156. M. Senske, L. Törk, B. Born, M. Havenith, C. Herrmann, S. Ebbinghaus
Protein stabilization by macromolecular crowding through enthalpy rather than entropy
J. Am. Chem. Soc. **136**, 9036–9041 (2014). DOI: 10.1021/ja503205y
155. K. Meister, J. Duman, Y. Xu, A. DeVries, D. Leitner, M. Havenith
The role of sulfates on antifreeze protein activity
J. Phys. Chem. B **118**, 7920–7924 (2014). DOI: 10.1021/jp5006742
154. M. Mischo, L. von Kobyletzki, E. Bründermann, D. Schmidt, A. Potthoff, N.H. Brockmeyer, M. Havenith
Similar appearance, different mechanisms: Xerosis in HIV, atopic dermatitis and aging
Exp. Dermatol. **23**, 446–448 (2014). DOI: 10.1111/exd.12425
153. E.T. Spielberg, E. Edengeiser, B. Mallick, M. Havenith, A.-V. Mudring
(1-Butyl-4-methyl-pyridinium)[Cu(SCN)₂]: A coordination polymer and ionic liquid
Chem. Eur. J. **20**, 5338–5345 (2014). DOI: 10.1002/chem.201302777
152. J. Sun, G. Niehues, H. Forbert, D. Decka, G. Schwaab, D. Marx, M. Havenith
Understanding THz spectra of aqueous solutions: Glycine in light and heavy water
J. Am. Chem. Soc. **136**, 5031–5038 (2014). DOI: 10.1021/ja4129857
151. P. Nieto, M. Letzner, T. Endres, G. Schwaab, M. Havenith
IR spectroscopy of pyridine-water conformers in helium nanodroplets
Phys. Chem. Chem. Phys. **16**, 8384–8391 (2014). DOI: 10.1039/c3cp55284e
150. H. Ogata, E. Decaneto, M. Grossman, M. Havenith, I. Sagi, W. Lubitz, M. Knipp
Crystallization and preliminary X-ray crystallographic analysis of the catalytic domain of membrane type 1 matrix metalloproteinase
Acta Cryst. **F70**, 232–235 (2014). DOI: 10.1107/S2053230X13034857
149. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith
Polarized 3D Raman and nanoscale near-field optical microscopy of optically inscribed surface relief gratings: chromophore orientation in azo-doped polymer films
Soft Matter **10**, 1544–1554 (2014). DOI: 10.1039/c3sm51787j
148. V.-S. Dang, H. Parala, J.H. Kim, K. Xu, N.B. Srinivasan, E. Edengeiser, M. Havenith, A.D. Wieck, T. de los Arcos, R.A. Fischer, A. Devi
Electrical and optical properties of TiO₂ thin films prepared by plasma-enhanced atomic layer deposition
Physica Status Solidi A **211**, 416–424 (2014). DOI: 10.1002/pssa.201330115
147. D. Peeters, G. Carraro, C. Maccato, H. Parala, A. Gasparatto, D. Barreca, C. Sada, K. Kartaschew, M. Havenith, D. Rogalla, H.-W. Becker, A. Devi
Tailoring iron (III) oxide nanomorphology by chemical vapor deposition: Growth and characterization
Physica Status Solidi A **211**, 316–322 (2014). DOI: 10.1002/pssa.201330079
146. J.-W. Lackmann, E. Edengeiser, S. Schneider, J. Benedikt, M. Havenith, J.E. Bandow
Effects of the effluent of a microscale atmospheric pressure plasma jet operated with He/O₂ gas on bovine serum albumin

- Plasma Medicine **3**, 115–124 (2013). DOI: 10.1615/PlasmaMed.2014008858
145. M. Letzner, S. Grün, D. Habig, K. Hanke, T. Endres, P. Nieto, G. Schwaab, Ł. Walewski, M. Wollenhaupt, H. Forbert, D. Marx, M. Havenith
High resolution spectroscopy of HCl–water clusters: IR bands of undissociated and dissociated clusters revisited
J. Chem. Phys. **139**, 154304 (2013). DOI: 10.1063/1.4824858
144. J.-W. Lackmann, S. Schneider, E. Edengeiser, F. Jarzina, S. Brinkmann, E. Steinborn, M. Havenith, J. Benedikt, J. Bandow
Photons and particles emitted from cold atmospheric-pressure plasma inactivate bacteria and biomolecules independently and synergistically
J. R. Soc. Interface **10**, 20130591 (2013). DOI: 10.1098/rsif.2013.0591
143. V. Sharma, F. Böhm, M. Seitz, G. Schwaab, M. Havenith
From solvated ions to ion-pairing: A THz study of lanthanum (III) hydration
Phys. Chem. Chem. Phys. **15**, 8383–8391 (2013). DOI: 10.1039/c3cp50865j
142. B. Born, M. Heyden, M. Grossman, I. Sagi, M. Havenith
Protein-water network dynamics during metalloenzyme hydrolysis observed by kinetic THz absorption (KITA)
Proceedings of SPIE **8585**, 85850E (2013). DOI: 10.1117/12.2000715
141. K. Meister, S. Ebbinghaus, Y. Xu, J.G. Duman, A. DeVries, M. Gruebele, D.M. Leitner, M. Havenith
Long-range protein-water dynamics in hyperactive insect antifreeze proteins
PNAS **110**, 1617–1622 (2013). DOI: 10.1073/pnas.1214911110
140. A. Patra, T.Q. Luong, R.K. Mitra, M. Havenith
Solvent dynamics in reverse micellar water-pool: A spectroscopic investigation of DDAB-cyclohexane-water systems
Phys. Chem. Chem. Phys. **15**, 930–939 (2013). DOI: 10.1039/c2cp42560b
139. D.M. Leitner, M. Gruebele, M. Havenith
THz technology and THz spectroscopy: Modeling and experiments to study solvation dynamics of biomolecules
In Methods in Physical Chemistry, Vol. 1, Wiley-VCH, 687–710 (2012).
DOI: 10.1002/9783527636839.ch22
138. L. von Kobyletzki, M. Mischo, D.A. Schmidt, E. Bründermann, N.H. Brockmeyer, A. Potthoff, M. Havenith
Probing epidermis and dermis by Raman spectroscopy: changes in antioxidant and lipid network with age and disease
Int. J. Cosmet. Sci. **34**, 372–373 (2012).
137. L. von Kobyletzki, M. Mischo, D.A. Schmidt, E. Bründermann, N.H. Brockmeyer, A. Potthoff, M. Havenith
Changes in antioxidant and lipid network in HIV patients compared to young and old patients: Probing epidermis and dermis by Raman spectroscopy
J. Dtsch. Dermatol. Ges. **10**, 15 (2012).
136. S. Funkner, M. Havenith, G. Schwaab
Urea, a structure breaker? Answers from THz absorption spectroscopy

- J. Phys. Chem. **116**, 13374–13380 (2012). DOI: 10.1021/jp308699w
135. M.A. Sliem, D.A. Schmidt, A. Betard, S.B. Kalidindi, S. Gross, M. Havenith, A. Devi, R.A. Fischer
Surfactant induced nonhydrolytic synthesis of phase-pure ZrO₂ nanoparticles from metal-organic and oxocluster precursors
Chem. Mat. **24**, 4274–4282 (2012). DOI: 10.1021/cm301128a
134. I. Kopf, H.W. Peindy N'Dongo, F. Ballout, U. Schatzschneider, E. Bründermann, M. Havenith
Introducing cymantrene labels into scattering scanning near-field infrared microscopy
Analyst **137**, 4995–5001 (2012). DOI: 10.1039/c2an16201f
133. J. Soetebier, M. Havenith
Der THz-Tanz des Wassers: Experimentelle Möglichkeiten der THz-Spektroskopie
GIT Labor-Fachzeitschrift **56**, 342–344 (2012)
132. B. Born, I. Sagi, M. Havenith
Water's contribution and enzyme's work – A KITA study
Proceedings of SPIE **8225**, 822518 (2012). DOI: 10.1117/12.907770
131. G. Niehues, A.L. Kaledin, J.M. Bowman, M. Havenith
Driving a small solvated peptide in the IR and THz range – A comparative study of energy flow
J. Phys. Chem. B **116**, 10020–10025 (2012). DOI: 10.1021/jp3021358
130. M. Heyden J. Sun, H. Forbert, G. Mathias, M. Havenith, D. Marx
Understanding the origins of dipolar couplings and correlated motion in the vibrational spectrum of water
J. Phys. Chem. Lett. **3**, 2135–2140 (2012). DOI: 10.1021/jz300748s
129. S. Ebbinghaus, K. Meister, M.B. Proghozin, A.L. DeVries, M. Havenith, J. Dzubiella, M. Gruebele
Functional importance of short-range binding and long-range solvent interactions in helical antifreeze peptides
Biophys. J. **103**, L20–L22 (2012). DOI: 10.1016/j.bpj.2012.06.013
128. N. Pérez-Hernández, T.Q. Luong, M. Febles, C. Marco, H.-H. Limbach, M. Havenith, C. Pérez, M.V. Roux, R. Pérez, J. Martín
The mobility of water molecules through hydrated pores
J. Phys. Chem. C **116**, 9616–9630 (2012). DOI: 10.1021/jp301323c
127. D.A. Schmidt, E. Bründermann, M. Havenith
Combined far- and near-field chemical nanoscope at ANKA-IR2: Applications and detection schemes
J. Phys.: Conf. Ser. **359**, 012015 (2012). DOI: 10.1088/1742-6596/359/1/012015
126. S. Funkner, G. Niehues, D.A. Schmidt, M. Heyden, G. Schwaab, K.M. Callahan, D.J. Tobias, M. Havenith
Watching the low frequency motions in aqueous salt solutions: The terahertz vibrational signatures of hydrated ions
J. Am. Chem. Soc. **134**, 1030–1035 (2012). DOI: 10.1021/ja207929u
125. A. Arora, T.Q. Luong, M. Krüger, Y.J. Kim, C.-H. Nam, A. Manz, M. Havenith
Terahertz-time domain spectroscopy for the detection of PCR amplified DNA in aqueous solution
Analyst **137**, 575–579 (2012). DOI: 10.1039/c2an15820e
(Cover article – <https://pubs.rsc.org/en/content/articlepdf/2012/an/c2an90002e>)

-
124. M. Havenith
Der THz-Tanz des Wassers mit den Proteinen
Biospektrum **17**, 38–41 (2011). DOI: 10.1007/s12268-011-0008-4
123. T.Q. Luong, P. Verma, R. Mitra, M. Havenith
Onset of hydrogen bonded collective network of water in 1,4-dioxane
J. Phys. Chem. A **115**, 14462–14469 (2011). DOI: 10.1021/jp204927r
122. F. Ballout, H. Krassen, I. Kopf, K. Ataka, E. Bründermann, J. Heberle, M. Havenith
Scanning near field IR microscopy of proteins in lipid bilayers
Phys. Chem. Chem. Phys. **13**, 21432–21436 (2011). DOI: 10.1039/c1cp21512d
121. T. Poerschke, D. Habig, M. Havenith
High resolution IR spectroscopy of the C-H stretch bands of benzene monomer and dimer in helium nanodroplets
Z. Phys. Chem. **225**, 1447–1456 (2011). DOI: 10.1524/zpch.2011.0193
120. M. Grossman, B. Born, M. Heyden, D. Tworowski, G.B. Fields, I. Sagi, M. Havenith
Correlated structural kinetics and retarded solvent dynamics at the metalloprotease active site
Nat. Struct. Mol. Biol. **18**, 1102–1108 (2011). DOI: 10.1038/nsmb.2120
See also: P. Ball, *More than a bystander*, Nature **478**, 467–468 (2011). DOI: 10.1038/478467a
119. M. Krüger, S. Funkner, E. Bründermann, M. Havenith
Uncertainty and ambiguity in terahertz parameter extraction and data analysis
J. Infrared Millim. Terahertz Waves **32**, 699–715 (2011). DOI: 10.1007/s10762-010-9669-1
118. G. Niehues, M. Heyden, D.A. Schmidt, M. Havenith
Exploring hydrophobicity by THz absorption spectroscopy of solvated amino acids
Faraday Discuss. **150**, 193–207 (2011). DOI: 10.1039/c0fd00007h
117. F. Ballout, J.-S. Samson, D.A. Schmidt, E. Bründermann, Y.-L. Mathis, B. Gasharova, A.D. Wieck, M. Havenith
Non-invasive nano-imaging of ion implanted and activated copper in silicon
J. Appl. Phys. **110**, 024307 (2011). DOI: 10.1063/1.3606415
116. T.Q. Luong, P.K. Verma, R.K. Mitra, M. Havenith
Do hydration dynamics follow the structural perturbation during thermal denaturation of a protein: A terahertz absorption study
Biophys. J. **101**, 925–933 (2011). DOI: 10.1016/j.bpj.2011.05.011
(Cover article)
115. M. Filimon, I. Kopf, D.A. Schmidt, E. Bründermann, J. Rühle, S. Santer, M. Havenith
Local chemical composition of nanophase-separated polymer brushes
Phys. Chem. Chem. Phys. **13**, 11620–11626 (2011). DOI: 10.1039/c0cp02756a
114. M. Krüger, M.-M. Huang, E. Bründermann, H. Weingärtner, M. Havenith
Combined THz and microwave dielectric spectroscopy of intermolecular interactions in homologous protic ionic liquids
IEEE Trans. Terahertz Sci. Technol. **1**, 313–320 (2011). DOI: 10.1109/TTHZ.2011.2159540
113. A. Metzelthin, E. Sánchez-García, Ö. Birer, G. Schwaab, W. Thiel, W. Sander, M. Havenith
Acetylene furan trimer formation at 0.37 K as a model for ultracold aggregation of non- and weakly polar molecules
ChemPhysChem **12**, 2009–2017 (2011). DOI: 10.1002/cphc.201001040

112. A. Gutberlet, G. Schwaab, M. Havenith
High resolution IR spectroscopy of dimers of HDO with H₂O in helium nanodroplets
J. Phys. Chem. A **115**, 6297–6305 (2011). DOI: 10.1021/jp201018x
111. M. Havenith
THz-Spektroskopie und Solvatationsdynamik
Nachrichten aus der Chemie **59**, 291–296 (2011). DOI: 10.1002/nadc.201176376

2006-2010

110. N. Zotov, M. Bartsch, L. Chernova, D.A. Schmidt, M. Havenith, G. Eggeler
Effects of annealing on the microstructure and the mechanical properties of EB-PVD thermal barrier coatings
Surf. Coat. Technol. **205**, 452–464 (2010). DOI: 10.1016/j.surfcoat.2010.07.008
109. M. Heyden, S. Ebbinghaus, M. Havenith
THz spectroscopy as a tool to study hydration dynamics
In: Encyclopedia of Analytical Chemistry: Applications, theory and instrumentation, Editor R.A. Meyers, Wiley-VCH (2010). DOI:10.1002/9780470027318.A9162
108. M. Heyden, M. Havenith
Combining THz spectroscopy and MD simulations to study protein-hydration coupling
Methods **52**, 74–83 (2010). DOI: 10.1016/j.ymeth.2010.05.007
107. A. Gutberlet, G. Schwaab, M. Havenith
High resolution IR spectroscopy of HDO and HDO-(N₂)_n in helium nanodroplets
J. Chem. Phys. **133**, 154313 (2010). DOI: 10.1063/1.3505054
106. S. Ebbinghaus, K. Meister, B. Born, A.L. DeVries, M. Gruebele, M. Havenith
Antifreeze glycoprotein activity correlates with long-range protein-water dynamics
J. Am. Chem. Soc. **132**, 12210–12211 (2010). DOI: 10.1021/ja1051632
105. M. Heyden, J. Sun, S. Funkner, G. Mathias, H. Forbert, M. Havenith, D. Marx
Dissecting the THz spectrum of liquid water from first principles via correlations in time and space
PNAS **107**, 12068–12073 (2010). DOI: 10.1073/pnas.0914885107
104. M.A. Sliem, T. Hikov, Z.-A. Li, M. Spasova, M. Farle, D.A. Schmidt, M. Havenith-Newen, R.A. Fischer
Interfacial Cu/ZnO contact by selective photodeposition of copper onto the surface of small ZnO nanoparticles in non-aqueous colloidal solution
Phys. Chem. Chem. Phys. **12**, 9858–9866 (2010). DOI: 10.1039/c003861j
103. M. Filimon, I. Kopf, F. Ballout, D.A. Schmidt, E. Bründermann, J. Rühle, S. Santer, M. Havenith
Smart polymer surfaces: Mapping chemical landscapes on the nanometre scale
Soft Matter **6**, 3764–3768 (2010). DOI: 10.1039/c0sm00098a
102. N. Pérez-Hernández, T.Q. Luong, C. Pérez, J.D. Martín, M. Havenith
Pore size dependent dynamics of confined water probed by FIR spectroscopy
Phys. Chem. Chem. Phys. **12**, 6928–6932 (2010). DOI: 10.1039/c000985g
101. M. Krüger, E. Bründermann, S. Funkner, H. Weingärtner, M. Havenith

- Communications: Polarity fluctuations of the protic ionic liquid ethylammonium nitrate in the terahertz regime*
J. Chem. Phys. **132**, 101101 (2010). DOI: 10.1063/1.3352585
100. K. Meister, D.A. Schmidt, E. Bründermann, M. Havenith
Confocal Raman microscopy as an analytical tool to assess the mitochondrial status in human spermatozoa
Analyst **135**, 1370–1374 (2010). DOI: 10.1039/b927012d
099. K. Meister, J. Niesel, U. Schatzschneider, N. Metzler-Nolte, D.A. Schmidt, M. Havenith
Label-free imaging of metal-carbonyl complexes in live cells by Raman microspectroscopy
Angew. Chem. Intl. Ed. **49**, 3310–3312 (2010). DOI: 10.1002/anie.201000097
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/anie.201001495>)
See also: P. Hildebrandt, *A spectral window to the cell*, Angew. Chem. Intl. Ed. **49**, 4540–4541 (2010). DOI: 10.1002/anie.201001616
098. E. Bründermann, D.A. Schmidt, I. Kopf, M. Havenith
Nano-spectroscopy and chemical nanoscopy of biomaterials
AIP Conf. Proc. **1214**, 7–9 (2010). DOI: 10.1063/1.3326355
097. S. Kundu, W. Xia, W. Busser, M. Becker, D.A. Schmidt, M. Havenith, M. Muhler
The formation of nitrogen-containing functional groups on carbon nanotube surfaces: A quantitative XPS and TPD study
Phys. Chem. Chem. Phys. **12**, 4351–4359 (2010). DOI: 10.1039/b923651a
096. I. Kopf, C. Grunwald, E. Bründermann, L. Casalis, G. Scoles, M. Havenith
Detection of hybridization on nanografted oligonucleotides using scanning near-field infrared microscopy
J. Phys. Chem. C **114**, 1306–1311 (2010). DOI: 10.1021/jp906813f
095. D.A. Schmidt, Ö. Birer, S. Funkner, B. Born, R. Gnanasekaran, G. Schwaab, D.M. Leitner, M. Havenith
Rattling in the cage: Ions as probes of sub- picosecond water network dynamics
J. Am. Chem. Soc. **131**, 18512–18517 (2009). DOI: 10.1021/ja9083545
094. B. Born, M. Havenith
Terahertz dance of proteins and sugars with water
J. Infrared Millim. Terahertz Waves **30**, 1245–1254 (2009). DOI: 10.1007/s10762-009-9514-6
093. A. Gutberlet, G. Schwaab, Ö. Birer, M. Masia, A. Kaczmarek, H. Forbert, M. Havenith, D. Marx
Aggregation induced dissociation of $\text{HCl}(\text{H}_2\text{O})_4$ below 1 K: The smallest droplet of acid
Science **324**, 1545–1548 (2009). DOI: 10.1126/science.1171753
See also:
T.S. Zwier, *Perspective: Squeezing the water out of $\text{HCl}(\text{aq})$*
Science **324**, 1522–1523 (2009). DOI: 10.1126/science.1175387
Nature research highlights, *Chemistry: The tiniest acid drop*
Nature **459**, 1036 (2009). DOI: 10.1038/4591036d
J. Urquhart, *Smallest acid droplet formed*
<https://www.chemistryworld.com/news/smallest-acid-droplet-formed/3003684.article>
092. J.-S. Samson, R. Meißner, E. Bründermann, M. Böke, J. Winter, M. Havenith
Characterization of single diamond-like and polymer-like nanoparticles by mid-infrared nanospectroscopy

- J. Appl. Phys. **105**, 064908 (2009). DOI: 10.1063/1.3086650
091. Ö. Birer, M. Havenith
High resolution infrared spectroscopy of formic acid dimer
Annu. Rev. Phys. Chem **60**, 263–275 (2009). DOI: 10.1146/annurev.physchem.040808.090431
090. B. Born, H. Weingärtner, E. Bründermann, M. Havenith
Solvation dynamics of model peptides probed by terahertz spectroscopy. Observation of the onset of collective network motions
J. Am. Chem. Soc. **131**, 3752–3755 (2009). DOI: 10.1021/ja808997y
089. E. Bründermann, I. Kopf, M. Havenith
Chemical nanoscopy of cell-like membranes
Proc. SPIE **7188**, 71880I (2009). DOI: 10.1117/12.808276
088. E. Bründermann, B. Born, S. Funkner, M. Krüger, M. Havenith
Terahertz spectroscopic techniques for the study of proteins in aqueous solutions
Proc. SPIE **7215**, 72150E (2009). DOI: 10.1117/12.808270
087. A.-S. Müller, T. Baumbach, S. Casalbuoni, B. Gasharova, M. Hagelstein, E. Huttel, Y.-L. Mathis, D.A. Moss, A. Plech, R. Rossmanith, E. Bründermann, M. Havenith, S. Hillenbrand, K.G. Sonnad
TBONE: Ultra-fast high-power coherent THz to mid-IR radiation facility
Proc. PAC09, TU5RFP028, 1156–1158 (2009)
086. B. Born, S.J. Kim, S. Ebbinghaus, M. Gruebele, M. Havenith
The terahertz dance of water with the proteins: The effect of protein flexibility on the dynamical hydration shell of ubiquitin
Faraday Discuss. **141**, 161–173 (2009). DOI: 10.1039/b804734k
085. A. Gutberlet, Ö. Birer, T. Poerschke, M. Havenith
High resolution infrared spectroscopy of the asymmetric C-H stretch of 1,2,4,5-Tetracyanobenzene (TCNB) and (TCNB)₂ in superfluid helium nanodroplets
J. Chem. Phys. **129**, 174311 (2008). DOI: 10.1063/1.2996356
084. A. Metzelthin, Ö. Birer, E. Sánchez-García, M. Havenith
High resolution IR-spectroscopy of acetylene-furan in ultracold helium nanodroplets
J. Chem. Phys. **129**, 114307 (2008). DOI: 10.1063/1.2976772
083. S.J. Kim, B. Born, M. Havenith, M. Gruebele
Echtzeitchweis von Änderungen im Protein-Wassernetzwerk während der Proteinfaltung mit Hilfe von Terahertz-Absorptionsspektroskopie
Angew. Chem. **120**, 6586–6589 (2008). DOI: 10.1002/ange.200802281
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/ange.200890220>)
082. S.J. Kim, B. Born, M. Havenith, M. Gruebele
Real-time detection of protein-water dynamics upon protein folding by terahertz absorption Spectroscopy
Angew. Chem. Int. Ed. **47**, 6486–6489 (2008). DOI: 10.1002/anie.200802281
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/anie.200890166>)
081. D.M. Leitner, M. Gruebele, M. Havenith
Solvation dynamics of biomolecules: Modeling and terahertz experiments
HFSP J. **2**, 314–323 (2008). DOI: 10.2976/1.2976661

080. K. Schröck, F. Schröder, M. Heyden, R.A. Fischer, M. Havenith
Characterization of interfacial water in MOF-5 ($\text{Zn}_4(\text{O})(\text{BDC})_3$)—a combined spectroscopic and theoretical study
Phys. Chem. Chem. Phys. **10**, 4732–4739 (2008). DOI: 10.1039/b807458P
079. G. Wollny, E. Bründermann, Z. Arsov, L. Quaroni, M. Havenith
Nanoscale depth resolution in scanning near-field infrared microscopy
Opt. Express **16**, 7453–7459 (2008). DOI: 10.1364/OE.16.007453
078. M. Heyden, E. Bründermann, U. Heugen, G. Niehues, D.M. Leitner, M. Havenith
Long range influence of carbohydrates on the solvation dynamics of water – Answers from THz absorption measurements and molecular modeling simulations
J. Am. Chem. Soc. **130**, 5773–5779 (2008). DOI: 10.1021/ja0781083
077. S. Ebbinghaus, S.J. Kim, M. Heyden, X. Yu, M. Gruebele, D.M. Leitner, M. Havenith
Protein sequence- and pH-dependent hydration probed by terahertz spectroscopy
J. Am. Chem. Soc. **130**, 2374–2375 (2008). DOI: 10.1021/ja0746520
076. E. Bründermann, M. Havenith
SNIM: Scanning near-field infrared microscopy
Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. **104**, 235–255 (2008). DOI: 10.1039/b703982b
(Cover article – <https://pubs.rsc.org/en/content/articlepdf/2008/pc/b807901n>)
075. A. Gutberlet, G.W. Schwaab, M. Havenith
High resolution IR spectroscopy of the carbonyl stretch of $(\text{DCOOD})_2$
Chem. Phys. **343**, 158–167 (2008). DOI: 10.1016/j.chemphys.2007.08.025
074. A. Metzelthin, M. Havenith
Observation of the $R(0.5) \ ^2\Pi_{1/2}$ transition in $^{15}\text{N}^{18}\text{O}$ in helium nanodroplets
Mol. Phys. **105**, 3025–3027 (2007). DOI: 10.1080/00268970701730104
073. S. Ebbinghaus, S.J. Kim, M. Heyden, X. Yu, U. Heugen, M. Gruebele, D.M. Leitner, M. Havenith
An extended dynamical solvation shell around proteins
PNAS **104**, 20749–20752 (2007). DOI: 10.1073/pnas.0709207104
072. M. Havenith
Schwingende Gerüste und tanzende Wassermoleküle
Nachrichten aus der Chemie **55**, 1090–1093 (2007). DOI: 10.1002/nadc.200751938
071. M. Ortlieb, Ö. Birer, M. Letzner, G.W. Schwaab, M. Havenith
Observation of rovibrational transitions of HCl, $(\text{HCl})_2$ and H_2O -HCl in liquid helium nanodroplets
J. Phys. Chem. A **111**, 12192–12199 (2007). DOI: 10.1021/jp0759980
070. M. Ortlieb, M. Havenith
Proton transfer in $(\text{HCOOH})_2$: An IR-high resolution spectroscopic study of the antisymmetric C-O stretch
J. Phys. Chem. A **111**, 7355–7363 (2007). DOI: 10.1021/jp070763+
069. M. Havenith, K. Kleinermanns, T. Koop
Physikalische Chemie des Wassers
Nachrichten aus der Chemie **55**, 285–288 (2007). DOI: 10.1002/nadc.200743720
068. I. Kopf, J.-S. Samson, G. Wollny, Ch. Grunwald, E. Bründermann, M. Havenith

- Chemical imaging of micro-structured self-assembled monolayers with nanometer resolution*
J. Phys. Chem. C **111**, 8166–8171 (2007). DOI: 10.1021/jp070201q
067. G.W. Schwaab, K. Schroeck, M. Havenith
Amplification of terahertz pulses in gases beyond thermodynamic equilibrium
Phys. Rev. A **75**, 032522 (2007). DOI: 10.1103/PhysRevA.75.032522
066. S. Rudolph, G. Wollny, K. von Haeften, M. Havenith
Probing collective excitations in helium nanodroplets: Observation of phonon wings in the infrared spectrum of methane
J. Chem. Phys. **126**, 124318 (2007). DOI: 10.1063/1.2709887
065. M. Havenith
Coherent proton tunneling in hydrogen bonds of isolated molecules: Carboxylic dimers
In: Hydrogen-Transfer Reactions, Editors J.T. Hynes, J.P. Klinman, H.-H. Limbach, R.L. Schowen, Wiley-VCH, 33–51 (2006). DOI: 10.1002/9783527611546.ch2
064. D.M. Leitner, M. Havenith M. Gruebele
Biomolecule large amplitude motion and solvation dynamics: Modeling and probes from THz to X-rays
Int. Rev. Phys. Chem. **25**, 553–582 (2006). DOI: 10.1080/01442350600862117
063. U. Heugen, G. Schwaab, E. Bründermann, M. Heyden, X. Yu, D.M. Leitner, M. Havenith
Solute-induced retardation of water dynamics probed directly by terahertz spectroscopy
PNAS **103**, 12301–12306 (2006). DOI: 10.1073/pnas.0604897103
062. M. Havenith, M. Ortlieb
Gefangen in der Quantenflüssigkeit
Physik in unserer Zeit **37**, 59 (2006). DOI: 10.1002/piuz.200690029
061. E. Bründermann, M. Havenith
Applications of semiconductor terahertz lasers in biomolecular spectroscopy and imaging
Proc. SPIE **6194**, 619406 (2006). DOI: 10.1117/12.673830
060. E. Bründermann, M. Havenith, G. Scalari, M. Giovanni, J. Faist, J. Kunsch, L. Mechold, M. Abraham
Turn-key compact high temperature terahertz quantum cascade lasers: Imaging and room temperature detection
Opt. Express **14**, 1829–1841 (2006). DOI: 10.1364/OE.14.001829
059. K. von Haeften, S. Rudolph, I. Simanowski, M. Havenith, R.E. Zillich, K.B. Whaley
Probing phonon-rotation coupling in Helium nanodroplets: Infrared spectroscopy of CO and its isotopomers
Phys. Rev. B **73**, 054502 (2006). DOI: 10.1103/PhysRevB.73.054502
058. J.-S. Samson, G. Wollny, E. Bründermann, A. Bergner, A. Hecker, G. Schwaab, A. D. Wieck, M. Havenith
Set-up of a scanning near field microscope (SNIM): Imaging of sub-surface nano-structures in gallium-doped silicon
Phys. Chem. Chem. Phys. **8**, 753–758 (2006). DOI: 10.1039/b512780g
057. S. Ebbinghaus, K. Schröck, J.C. Schauer, E. Bründermann, M. Heyden, G. Schwaab, M. Böke, J. Winter, M. Tani, M. Havenith

Terahertz time-domain spectroscopy as a new tool for the characterization of dust forming plasmas

Plasma Sources Sci. Technol. **15**, 72–77 (2006). DOI: 10.1088/0963-0252/15/1/011

2001-2005

056. K. von Haeften, A. Metzelthin, S. Rudolph, V. Staemmler, M. Havenith
High resolution spectroscopy of NO in helium droplets: A prototype for open shell molecular interactions in a quantum solvent
Phys. Rev. Lett. **95**, 215301 (2005). DOI: 10.1103/PhysRevLett.95.215301
055. M. Havenith, G.W. Schwaab
Attacking a small beast: Ar-CO, a prototype for intermolecular forces
Z. Phys. Chem. **219**, 1053–1088 (2005). DOI: 10.1524/zpch.2005.219.8.1053
054. A. Bergner, U. Heugen, E. Bründermann, G. Schwaab, M. Havenith, D.R. Chamberlin, E.E. Haller
New p-Ge THz spectrometer for the study of solutions: THz absorption spectroscopy of water
Rev. Sci. Instr. **76**, 063110 (2005). DOI: 10.1063/1.1928427
053. E. Bründermann, U. Heugen, R. Schiwon, B. Born, G.W. Schwaab, S. Ebbinghaus, K. Schröck, D.R. Chamberlin, E.E. Haller, M. Havenith
Terahertz imaging applications in spectroscopy of biomolecules
IEEE MTT-S International Microwave Symposium Digest, 625–628 (2005).
DOI: 10.1109/MWSYM.2005.1516679
052. R. Schiwon, G. Schwaab, E. Bründermann, M. Havenith
Terahertz cavity enhanced attenuated total reflection spectroscopy
Appl. Phys. Lett. **86**, 201116 (2005). DOI: 10.1063/1.1929072
051. K. von Haeften, M. Havenith
He droplets: A fluid with unusual properties
In: Electronic excitations in liquefied rare gases, Editors W.F. Schmidt and E. Illenberger, American Scientific Publishers (2005).
050. E. Bründermann, A. Bergner, F. Petrat, R. Schiwon, G. Wollny, I. Kopf, H. de Groot, M. Havenith
Fast quantification of water in single living cells by near-infrared microscopy
Analyst **129**, 893–896 (2004). DOI: 10.1039/B408954P
049. S. Hoffmann, M. Hofmann, E. Bründermann, M. Havenith, M. Matus, J.V. Moloney, A.S. Moskalenko, M. Kira, S.W. Koch, S. Saito, K. Sakai
Four-wave mixing and direct terahertz emission with two-color semiconductor lasers
Appl. Phys. Lett. **84**, 3585–3587 (2004). DOI: 10.1063/1.1737486
048. R.A. Jockusch, R.T. Kroemer, F.O. Talbot, L.C. Snoek, P. Çarçabal, J.P. Simons, M. Havenith, J.M. Bakker, I. Compagnon, G. Meijer, G. von Helden
Probing the glycosidic linkage: UV and IR ion-dip spectroscopy of lactoside
J. Am. Chem. Soc. **126**, 5709–5714 (2004). DOI: 10.1021/ja031679k
047. F. Madeja, M. Havenith, K. Nauta, R.E. Miller, J. Chocholoušová, P. Hobza
Polar isomer of formic acid dimer formed in helium nano-droplets
J. Chem. Phys. **120**, 10554–10560 (2004). DOI: 10.1063/1.1709942
046. R. Schiwon, G.W. Schwaab, E. Bründermann, M. Havenith

- Far-infrared multilayer mirrors*
Appl. Phys. Lett. **83**, 4119–4121 (2003). DOI: 10.1063/1.1627479
045. M. Havenith
Comment on: Theoretical absorption spectrum of the Ar-CO van der Waals complex [J. Chem. Phys. 118, 9596 (2003)]
J. Chem. Phys. **119**, 7604 (2003). DOI: 10.1063/1.1606671
044. I. Scheele, M. Havenith
High-resolution IR spectroscopy of a high lying $K_a = 0$ mode of the weakly bound van der Waals complex Ar-CO
Mol. Phys. **101**, 1423–1427 (2003). DOI: 10.1080/0026897031000092265
043. F. Madeja, A. Hecker, S. Ebbinghaus, M. Havenith
High resolution spectroscopy of ν_3 band of the van der Waals complex Ar-DCOOH
Mol. Phys. **101**, 1511–1515 (2003). DOI: 10.1080/0026897031000108078
042. A. Hecker, I. Scheele, M. Havenith
IR-High resolution spectroscopy of the N_2O dimer: The torsional mode
Phys. Chem. Chem. Phys. **5**, 2333–2336 (2003). DOI: 10.1039/b300733m
041. M. Havenith, B.A. Hess
Weakly interacting molecular complexes
In: Interactions in molecules: Electronic and steric effects (final report of the Collaborative Research Centre 334), Editor S.D. Peyerimhoff, Wiley-VCH, 110–131 (2003).
040. F. Madeja, A. Hecker, S. Ebbinghaus, M. Havenith
High resolution spectroscopy of ν_3 band of DCOOD
Spectrochim. Acta A **59**, 1773–1782 (2003). DOI: 10.1016/S1386-1425(02)00412-2
039. A. Hecker, M. Havenith, C. Braxmaier, U. Strößner, A. Peters
High resolution Doppler-free spectroscopy of molecular iodine using a continuous wave optical parametric oscillator
Opt. Commun. **218**, 131–134 (2003). DOI: 10.1016/S0030-4018(03)01187-8
038. N. Pörtner, A.F. Vilesov, M. Havenith
Spontaneous alignment of tetracene molecules in ^4He droplets
Chem. Phys. Lett. **368**, 458–464 (2003). DOI: 10.1016/S0009-2614(02)01903-6
037. G. Gimmler, M. Havenith
High-resolution IR-spectroscopy of the N_2O - H_2O and N_2O - D_2O van der Waals complexes
J. Mol. Spec. **216**, 315–321, (2002). DOI: 10.1006/jmsp.2002.8687
036. F. Madeja, M. Havenith
High resolution spectroscopy of carboxylic acid in the gas phase: Observation of proton transfer in $(\text{DCOOH})_2$
J. Chem. Phys. **117**, 7162–7168 (2002). DOI: 10.1063/1.1507581
035. M. Kunze, P. Markwick, N. Pörtner, J. Reuss, M. Havenith
IR-MW double resonance spectroscopy of OCS in pure ^4He and mixed $^4\text{He}/^3\text{He}$ clusters
J. Chem. Phys. **116**, 7473–7485 (2002). DOI: 10.1063/1.1467330
034. F. Madeja, P. Markwick, M. Havenith, K. Nauta, R.E. Miller

Rotationally resolved infrared spectroscopy of h_2 - and d_1 -formic acid monomer in liquid He-droplets

J. Chem. Phys. **116**, 2870–2878 (2002). DOI: 10.1063/1.1432998

033. M. Havenith

Infrared spectroscopy of molecular clusters: An introduction to intermolecular forces

Springer Tracts in Modern Physics **176**, Springer-Verlag Berlin Heidelberg (2002).

DOI: 10.1007/3-540-45457-8

032. N. Pörtner, A.F. Vilesov, M. Havenith

The formation of heterogeneous van der Waals complexes in helium droplets

Chem. Phys. Lett. **343**, 281–288 (2001). DOI: 10.1016/S0009-2614(01)00648-0

031. G. Gimmler, M. Havenith

Free-jet infrared diode laser spectroscopy of the ν_2 -band of the Ar- N_2O van der Waals complex

J. Mol. Struct. **599**, 117–123 (2001). DOI: 10.1016/S0022-2860(01)00840-7

030. I. Scheele, R. Lehnig, M. Havenith

IR spectroscopy of van der Waals modes in the intermolecular potential of Ar-CO: The $K_a = 0$ combination of stretch and bending

Mol. Phys. **99**, 197–203 (2001). DOI: 10.1080/00268970010007587

029. I. Scheele, R. Lehnig, M. Havenith

Observation of a high lying van der Waals mode in the intermolecular potential of Ar-CO

Mol. Phys. **99**, 205–209 (2001). DOI: 10.1080/00268970010008351

1988-2000

028. S. Grebenev, M. Havenith, F. Madeja, J.P. Toennies, A.F. Vilesov

Microwave-infrared double resonance spectroscopy of OCS molecules inside a ^4He droplet

J. Chem. Phys. **113**, 9060–9066 (2000). DOI: 10.1063/1.1286243

027. S. Grebenev, M. Hartmann, M. Havenith, B. Sartakov, J.P. Toennies, A.F. Vilesov

The rotational spectrum of single OCS molecules in liquid ^4He droplets

J. Chem. Phys. **112**, 4485–4495 (2000). DOI: 10.1063/1.481011

026. U. Merker, P. Engels, F. Madeja, M. Havenith, W. Urban

High-resolution CO-laser sideband spectrometer for molecular-beam optothermal spectroscopy in the 5-6.6 μm wavelength region

Rev. Sci. Instr. **70**, 1933–1938 (1999). DOI: 10.1063/1.1149691

025. C. Schmidt, M. Perić, P. Mürtz, M. Wienkoop, M. Havenith, W. Urban

Faraday laser magnetic resonance spectroscopy of vibrationally excited C_2D

J. Mol. Spec. **190**, 112–124 (1998). DOI: 10.1006/jmsp.1998.7563

024. M. Scherer, M. Havenith, R. Mausberger, T.L. Wilson

A search for $(\text{H}_2\text{O})_2$ in the galaxy and toward comet Hale-Bopp

Astron. Astrophys. **335**, 1070–1076 (1998).

023. M. Wienkoop, P. Mürtz, P.-C. Schumann, M. Havenith, W. Urban

First observation of ro-vibrational transitions of the SiC radical by infrared LMR spectroscopy

Chem. Phys. **225**, 17–21 (1997). DOI: 10.1016/S0301-0104(97)00199-7

022. M. Behrens, U. Buck, R. Fröchtenicht, M. Hartmann, M. Havenith

- The ammonia dimer spectrum in cold helium clusters*
J. Chem. Phys. **107**, 7179–7186 (1997). DOI: 10.1063/1.474957
021. S. König, M. Havenith
Measurement of the $K_a=1$ ($v_{CO}=1$) stretching mode in Ar-CO using a Herriott multipass cell
Mol. Phys. **91**, 265–272 (1997). DOI: 10.1080/002689797171571
020. Y. Xu, S. Civiš, R. McKellar, S. König, M. Haverlag, G. Hilpert, M. Havenith
High K ("Propeller") states in the infrared spectrum of the Ar-CO complex
Mol. Phys. **87**, 1071–1082 (1996). DOI: 10.1080/00268979600100741
019. C. Pfelzer, M. Havenith, M. Perić, P. Mürtz, W. Urban
Faraday laser magnetic resonance spectroscopy on vibrational excited C_2H
J. Mol. Spec. **176**, 28–37 (1996). DOI: 10.1006/jmsp.1996.0058
018. S. König, G. Hilpert, M. Havenith
Observation of strong Coriolis coupling in the IR spectrum of Ar-CO
Mol. Phys. **86**, 1233–1247 (1995). DOI: 10.1080/00268979500102701
017. B. Meyer, S. Saupe, M.H. Wappelhorst, T. George, F. Kühnemann, M. Schneider, M. Havenith, W. Urban, J. Legrand
CO laser sideband spectrometer: Sub-Doppler heterodyne frequency measurements around 5 μm
Appl. Phys. B **61**, 169–173 (1995). DOI: 10.1007/BF01090939
016. H. Linnartz, M. Havenith, W.L. Meerts
The ammonia dimer: Complex dynamics with a dynamical complex
Com. At. Mol. Phys. **30**, 315–329 (1995).
015. N. Heineking, W. Stahl, E.H.T. Olthof, P.E.S. Wormer, A. van der Avoird, M. Havenith
The nuclear quadrupole coupling constants and the structure of the para-para ammonia dimer
J. Chem. Phys. **102**, 8693–8703 (1995). DOI: 10.1063/1.468972
014. H. Linnartz, W.L. Meerts, M. Havenith
The ammonia dimer: New infrared–far-infrared double resonance results
Chem. Phys. **193**, 327–338 (1995). DOI: 10.1016/0301-0104(94)00413-5
013. M. Havenith, M. Petri, C. Lubina, G. Hilpert, W. Urban
IR spectroscopy of $(CO)_2$ using concentration frequency double modulation in a supersonic expansion
J. Mol. Spec. **167**, 248–261 (1995). DOI: 10.1006/jmsp.1994.1232
012. G. Hilpert, H. Linnartz, M. Havenith, J.J. ter Meulen, W.L. Meerts
Tunable infrared and far-infrared direct absorption spectroscopy of molecular ions in a supersonic jet expansion
Chem. Phys. Lett. **219**, 384–388 (1994). DOI: 10.1016/0009-2614(94)00129-4
011. M. Havenith, G. Hilpert, M. Petri, W. Urban
Measurement of the first excited bending state of Ar-CO using a new concentration modulation technique in the jet
Mol. Phys. **81**, 1003–1010 (1994). DOI: 10.1080/00268979400100661
010. H. Linnartz, A. Kips, W.L. Meerts, M. Havenith
The electric dipole moment of $(NH_3)_2$ for $G: ||K||=1$

- J. Chem. Phys. **99**, 2449–2452 (1993). DOI: 10.1063/1.465208
009. M. Havenith, H. Linnartz, E. Zwart, A. Kips, J.J. ter Meulen, W.L. Meerts
An infrared–far-infrared double resonance study on $(\text{NH}_3)_2$ in a jet
Chem. Phys. Lett. **193**, 261–268 (1992). DOI: 10.1016/0009-2614(92)85665-W
008. H. Linnartz, M. Havenith, E. Zwart, W.L. Meerts, J.J. ter Meulen
The determination of the electric dipole moment of KrH^+
J. Mol. Spec. **153**, 710–717 (1992). DOI: 10.1016/0022-2852(92)90505-I
007. M. Havenith, M. Schneider, W. Bohle, W. Urban
Sub-Doppler Faraday LMR spectroscopy: First applications to NO and DBr^+
Mol. Phys. **72**, 1149–1158 (1991). DOI: 10.1080/00268979100100821
006. M. Havenith, R.C. Cohen, K.L. Busarow, D.-H. Gwo, Y.T. Lee, R.J. Saykally
Measurement of the intermolecular vibration-rotation-tunneling spectrum of the ammonia dimer by tunable far infrared laser spectroscopy
J. Chem. Phys. **94**, 4776–4789 (1991). DOI: 10.1063/1.460562
005. M. Havenith, E. Zwart, W.L. Meerts, J.J. ter Meulen
Determination of the dipole moment of HN_2^+
J. Chem. Phys. **93**, 8446–8451 (1990). DOI: 10.1063/1.459282
004. D.-H. Gwo, M. Havenith, K.L. Busarow, R.C. Cohen, Ch.A. Schmuttenmaer, R.J. Saykally
Tunable far infrared laser spectroscopy of van der Waals bonds: The $J_{\text{KC}} = 1_0 \leftarrow 0_0 \Sigma$ bending vibration of $\text{Ar-}^{14}\text{NH}_3$
Mol. Phys. **71**, 453–460 (1990). DOI: 10.1080/00268979000101901
003. W. Urban, J.-X. Lin, V.V. Subramaniam, M. Havenith, J.W. Rich
Treanor pumping of CO initiated by CO laser excitation
Chem. Phys. **130**, 389–399 (1989). DOI: 10.1016/0301-0104(89)87068-5
002. R.C. Cohen, K.L. Busarow, K.B. Laughlin, G.A. Blake, M. Havenith, Y.T. Lee, R.J. Saykally
Tunable far infrared laser spectroscopy of van der Waals bonds: Vibration-rotation-tunneling spectra of $\text{Ar-H}_2\text{O}$
J. Chem. Phys. **89**, 4494–4504 (1988). DOI: 10.1063/1.454789
001. M. Havenith, W. Bohle, J. Werner, W. Urban
Vibration rotation spectroscopy of excited electronic states: Faraday-L.M.R. spectroscopy of $\text{CO } a^3\pi$
Mol. Phys. **64**, 1073–1088 (1988). DOI: 10.1080/00268978800100723
-