Publications by Dominik Marx

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Lehrstuhl für Theoretische Chemie, Ruhr–Universität Bochum; March 18, 2024

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1 Peer Reviewed Publications

[291] A. Jindal, P. Schienbein, and D. Marx,
Revealing the Molecular Origin of Anisotropy around Chloride Ions in Bulk Water,
J. Phys. Chem. Lett. **15**, 3037–3042 (2024);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2024-15-3037.pdf>`
with 15 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2024-15-3037-si.pdf>`

[290] S. Maste, B. Sharma, T. Pongratz, B. Grabe, W. Hiller, M. Beck Erlach, W. Kremer, H. R. Kalbitzer, D. Marx, and S. M. Kast,
The accuracy limit of chemical shift predictions for species in aqueous solution,
Phys. Chem. Chem. Phys. **26**, 6386–6395 (2024);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2024-26-6386.pdf>`
with 12 pages of Electronic Supplementary Material;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2024-26-6386-si.pdf>`
with raw research data provided open-access via RESOLV RDM.
`https://doi.org/10.17877/RESOLV-2024-lrgkievk`

[289] S. Ruiz–Barragan, H. Forbert, and D. Marx,
Anisotropic pressure effects on nanoconfined water within narrow graphene slit pores,
Phys. Chem. Chem. Phys. **25**, 28119–28129 (2023).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2023-25-28119.pdf>`

[288] F. Brieuc, C. Schran, and D. Marx,
Manifestations of local supersolidity of ^{4}He around a charged molecular impurity,
Phys. Rev. Res. **5**, 043083-1-19 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRR-2023-5-043083.pdf>`
with 68 pages of Supplemental Material (nnp-parameters.pdf file).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRR-2023-5-043083-SI.pdf>`

[287] I. Simko, C. Schran, F. Brieuc, C. Fabri, O. Asvany, S. Schlemmer, D. Marx, and A. G. Csaszar,
Quantum Nuclear Delocalization and its Rovibrational Fingerprints,
Angew. Chem. Int. Ed. **62**, e202306744 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie202306744.pdf>`
with 15 pages of Supporting Information and NNP Parameter File.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie202306744-si.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie202306744-nnp.pdf>`

[286] A. Gulzar, J. Noetzel, H. Forbert, and D. Marx,
Elucidating the Self-cleavage Dynamics of Hairpin Ribozyme by Mode-decomposed

Infrared Spectroscopy,
J. Phys. Chem. Lett. **14**, 7940–7945 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2023-14-7940.pdf>`
with 17 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2023-14-7940-si.pdf>`

[285] V. A. Tran, M. Teucher, L. Galazzo, B. Sharma, T. Pongratz, S. M. Kast, D. Marx, E. Bordignon, A. Schnegg, and F. Neese,
Dissecting the Molecular Origin of g-Tensor Heterogeneity and Strain in Nitroxide Radicals in Water: Electron Paramagnetic Resonance Experiment versus Theory,
J. Phys. Chem. A **127**, 6447–6466 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca-2023-127-6447.pdf>`
with 17 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca-2023-127-6447-si.pdf>`

[284] R. Beckmann, R. Topolnicki, and D. Marx,
Deciphering the Impact of Helium Tagging on Flexible Molecules: Probing Microsolvation Effects of Protonated Acetylene by Quantum Configurational Entropy,
J. Phys. Chem. A **127**, 2460–2471 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca-2023-127-2460.pdf>`
with 14 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca-2023-127-2460-si.pdf>`

[283] S. Tsuru, B. Sharma, D. Marx, and C. Hättig,
Structural Sampling and Solvation Models for the Simulation of Electronic Spectra: Pyrazine as a Case Study,
J. Chem. Theory Comput. **19**, 2291–2303 (2023).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-2023-19-2291.pdf>`

[282] J. A. Davies, C. Schran, F. Brieuc, D. Marx, and A. M. Ellis,
Onset of Rotational Decoupling for a Molecular Ion Solvated in Helium: From Tags to Rings and Shells,
Phys. Rev. Lett. **130**, 083001-1–6 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2023-130-083001.pdf>`
with 17 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2023-130-083001-SI.pdf>`

[281] B. Das, S. Ruiz–Barragan, and D. Marx,
Deciphering the Properties of Nanoconfined Aqueous Solutions by Vibrational Sum Frequency Generation Spectroscopy,
J. Phys. Chem. Lett. **14**, 1208–1213 (2023);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2023-14-1208.pdf>`
with 21 pages of Supporting Information;

Anonymous ftp: <outgoing/dominik_marx/PAPERS/jpcl-2023-14-1208-si.pdf>
see also *Cover Picture*.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jpcl-2023-14-1208-cover.pdf>

[280] J. Daru, H. Forbert, J. Behler, and D. Marx,
Coupled Cluster Molecular Dynamics of Condensed Phase Systems Enabled by Machine Learning Potentials: Liquid Water Benchmark,
Phys. Rev. Lett. **129**, 226001-1–6 (2022);
The PRL Editors: We have selected your recently accepted manuscript to be a PRL Editors' Suggestion. About one Letter in six is chosen for this highlighting. We look for papers that we judge to be particularly important, interesting, and well written.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prl-2022-129-226001.pdf>
with 21 pages of Supplemental Material;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prl-2022-129-226001-si.pdf>
see also coverage in the media:
T. D. Kühne, Dem Wasser auf der Spur, Physik Journal **22**, 22–23 (2023).

[279] S. Ruiz–Barragan, F. Sebastiani, P. Schienbein, J. Abraham, G. Schwaab, R. R. Nair, M. Havenith, and 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);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2022-24-24734.pdf>
with 17 pages of Electronic Supplementary Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2022-24-24734-si.pdf>

[278] H. R. Larsson, M. Schröder, R. Beckmann, F. Brieuc, C. Schran, D. Marx, and O. Vendrell,
State-resolved infrared spectrum of the protonated water dimer: revisiting the characteristic proton transfer doublet peak,
Chem. Sci. **13**, 11119–11125 (2022);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/chemsci-2022-13-11119.pdf>
with 7 pages of Electronic Supplementary Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/chemsci-2022-13-11119-si.pdf>

[277] R. Beckmann, F. Brieuc, C. Schran, and D. Marx,
Infrared Spectra at Coupled Cluster Accuracy from Neural Network Representations,
J. Chem. Theory Comput. **18**, 5492–5501 (2022);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jctc-2022-18-5492.pdf>
with Supporting Information data (zip file).
https://pubs.acs.org/doi/10.1021/acs.jctc.2c00511

[276] L. Duran Caballero, C. Schran, F. Brieuc, and D. Marx,
Neural network interaction potentials for para-hydrogen with flexible molecules,
J. Chem. Phys. **157**, 074302-1–12 (2022);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2022-157-074302.pdf>`
with 24 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2022-157-074302-SI.pdf>`

[275] D. Mani, T. K. Roy, J. Khatri, G. Schwaab, S. Blach, C. Hölzl, H. Forbert, D. Marx, and M. Havenith,
Internal Electric Field-Induced Formation of Exotic Linear Acetonitrile Chains,
J. Phys. Chem. Lett. **13**, 6852–6858 (2022);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2022-13-6852.pdf>`
with 52 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2022-13-6852-si.pdf>`
see also *Cover Picture.*
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2022-13-6852-cover.jpg>`

[274] J. Noetzel, P. Schienbein, H. Forbert, and D. Marx,
Solvation of small gold clusters in supercritical water,
J. Mol. Liq. **362**, 119715-1–10 (2022);
part of the "Gábor Pálinkás Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JML-2022-362-119715.pdf>`
`https://www.sciencedirect.com/journal/journal-of-molecular-liquids/special-issue/10FRT2RBJ0R`

[273] G. Schwaab, R. Perez de Tudela, D. Mani, N. Pal, T. Kumar Roy, F. Gabas, R. Conte, L. Duran Caballero, M. Ceotto, D. Marx, and M. Havenith,
Zwitter Ionization of Glycine at Outer Space Conditions due to Microhydration by Six Water Molecules,
Phys. Rev. Lett. **128**, 033001-1–6 (2022);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2022-128-033001.pdf>`
with 26 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2022-128-033001-SI.pdf>`

[272] J. Thomas, C. Bertram, J. Daru, J. Patwari, I. Langguth, P. Zhou, D. Marx, K. Morgenstern, and U. Bovensiepen,
Competition between Coulomb and van der Waals Interactions in Xe–Cs^+ Aggregates on Cu(111) Surfaces,
Phys. Rev. Lett. **127**, 266802-1–6 (2021);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2021-127-266802.pdf>`
with 9 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2021-127-266802-SI.pdf>`

[271] B. Sharma, V. A. Tran, T. Pongratz, L. Galazzo, I. Zhurko, E. Bordignon, S. M. Kast, F. Neese, and D. Marx,
A Joint Venture of Ab Initio Molecular Dynamics, Coupled Cluster Electronic Structure Methods, and Liquid State Theory to Compute Accurate Isotropic Hyperfine Constants of Nitroxide Probes in Water,
J. Chem. Theory Comput. **17**, 6366–6386 (2021);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-2021-17-6366.pdf>`
with 8 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-2021-17-6366-si.pdf>`
see also *Cover Picture*.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-2021-17-6366-cover.pdf>`

[270] C. Hölzl, H. Forbert, and D. Marx,
Dielectric Relaxation of Water: Assessing the Impact of Localized Modes, Translational Diffusion, and Collective Dynamics,
Phys. Chem. Chem. Phys. **23**, 20875–20882 (2021).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2021-23-20875.pdf>`

[269] 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, and M. Havenith
Aqueous TMAO solution under high hydrostatic pressure,
Phys. Chem. Chem. Phys. **23**, 11355–11365 (2021);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2021-23-11355.pdf>`
with 31 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2021-23-11355-si.pdf>`

[268] R. Tripathi, L. Duran Caballero, R. Perez de Tudela, C. Hölzl, and D. Marx,
Unveiling Zwitterionization of Glycine in the Microhydration Limit,
ACS Omega **6**, 12676–12683 (2021);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acso-2021-6-12676.pdf>`
with 21 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acso-2021-6-12676-si.pdf>`

[267] F. Sebastiani, C. Y. Ma, S. Funke, A. Bäumer, D. Decka, C. Hoberg, A. Esser, H. Forbert, G. Schwaab, D. Marx, and M. Havenith,
Probing Local Electrostatics of Glycine in Aqueous Solution by THz Spectroscopy,
Angew. Chem. Int. Ed. **60**, 3768–3772 (2021);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-202014133.pdf>`
with 20 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-202014133-si.pdf>`

[266] C. Schran, F. Brieuc, and D. Marx,
Communication: Transferability of machine learning potentials: Protonated water

neural network potential applied to the protonated water hexamer,
J. Chem. Phys. **154**, 051101-1–6 (2021).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2021-154-051101.pdf>`

[265] D. H. Patel, D. Marx, and A. L. L. East,
Improving the Yield and Rate of Acid-Catalyzed Deconstruction of Lignin by Mechanochemical Activation,
ChemPhysChem **21**, 2660–2666 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2020-21-2660.pdf>`
with 54 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2020-21-2660-SI.pdf>`

[264] P. Dopieralski, M. E. Zoloff Michoff, and D. Marx,
Mechanochemical disulfide reduction reveals imprints of noncovalent sulfur$\cdots$oxygen chalcogen bonds in protein-inspired mimics in aqueous solution,
Phys. Chem. Chem. Phys. **22**, 25112–25117 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2020-22-25112.pdf>`
with 17 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2020-22-25112-si.pdf>`

[263] R. Topolnicki, F. Brieuc, C. Schran, and D. Marx,
Deciphering High-Order Structural Correlations within Fluxional Molecules from Classical and Quantum Configurational Entropy,
J. Chem. Theory Comput. **16**, 6785–6794 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-0c00642.pdf>`
with 29 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-0c00642-si.pdf>`

[262] N. Kumar and D. Marx,
On the Adaptability of the Chemical Reaction of Hairpin Ribozyme to High Pressures,
J. Phys. Chem. Lett. **11**, 92998–9303 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2020-11-9298.pdf>`
with 20 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2020-11-9298-si.pdf>`

[261] A. A. Auer, V. A. Tran, B. Sharma, G. L. Stoychev, D. Marx, and F. Neese,
A case study of density functional theory and domain-based local pair natural orbital coupled cluster for vibrational effects on EPR hyperfine coupling constants: vibrational perturbation theory versus ab initio *molecular dynamics,*
Mol. Phys. **118**, e1797916-1–16 (2020).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/MolPhys-2020-118-1797916.pdf>`

[260] P. Schienbein and D. Marx,
Supercritical Water is not Hydrogen Bonded,
Angew. Chem. Int. Ed. **59**, 18578–18585 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-202011869.pdf>`
with 32 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-202011869-si.pdf>`
see also *Cover Picture.*
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-202011869-cover.pdf>`
Featured as a *"Very Important Paper" (VIP)*;
see also coverage in the media:
M. Tolan, Wasser ohne Brücken, Physik Journal **19**, 18–19 (2020);
P. Ball, Simulation says supercritical water has no hydrogen bonds,
Chemistry World 48–48, October 2020.

[259] S. Imoto and D. Marx,
How Can Protons Migrate in Extremely Compressed Liquid Water?
Phys. Rev. Lett. **125**, 086001-1–6 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2020-125-086001.pdf>`
with 14 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2020-125-086001-SI.pdf>`

[258] N. Siemer, D. Munoz-Santiburcio, and D. Marx,
Solvation-Enhanced Oxygen Activation at Gold/Titania Nanocatalysts,
ACS Catal. **10**, 8530–8534 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acscatal.0c01326.pdf>`
with 18 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acscatal.0c01326-si.pdf>`
See also *ACS Catalysis Tweet:*
`https://twitter.com/ACSCatalysis/status/1288044212328554497`

[257] N. Kumar and D. Marx,
Deciphering the Self-Cleavage Reaction Mechanism of Hairpin Ribozyme,
J. Phys. Chem. B **124**, 4906–4918 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acs.jpcb.0c03768.pdf>`
with 8 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acs.jpcb.0c03768-si.pdf>`

[256] S. Ruiz–Barragan, D. Munoz–Santiburcio, S. Körning, and D. Marx,
Communication: Quantifying anisotropic dielectric response properties of nanoconfined water within graphene slit pores,
Phys. Chem. Chem. Phys. **22**, 10833–10837 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2020-22-10833.pdf>`

with 18 pages of Electronic Supplementary Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2020-22-10833-si.pdf>

[255] R. Perez de Tudela and D. Marx,
Generating Excess Protons in Microsolvated Acid Clusters under Ambient Conditions: An Issue of Configurational Entropy versus Internal Energy,
Chem. Eur. J. **26**, 11955–11959 (2020);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CEJ-2020-26-11955.pdf>
with 4 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CEJ-2020-26-11955-SI.pdf>

[254] P. Schienbein and D. Marx,
Assessing the properties of supercritical water in terms of structural dynamics and electronic polarization effects,
Phys. Chem. Chem. Phys. **22**, 10462–10479 (2020);
part of the "Michiel Sprik Festschrift": Frontiers in Molecular Simulation of Solvated Ions, Molecules and Interfaces;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2020-22-10462.pdf>
with 7 pages of Electronic Supplementary Material and 28 files containing digital data.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2020-22-10462-si.pdf>

[253] C. Schran, J. Behler, and D. Marx,
Automated Fitting of Neural Network Potentials at Coupled Cluster Accuracy: Protonated Water Clusters as Testing Ground,
J. Chem. Theory Comput. **16**, 88–99 (2020);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jctc-9b00805.pdf>
with 40 pages of Supporting Information;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jctc-9b00805-si.pdf>

[252] T. Pongratz, P. Kibies, L. Eberlein, N. Tielker, C. Hölzl, S. Imoto, M. Beck Erlach, S. Kurrmann, P. H. Schummel, M. Hofmann, O. Reiser, R. Winter, W. Kremer, H. R. Kalbitzer, D. Marx, D. Horinek, and S. M. Kast,
Pressure-dependent electronic structure calculations using integral equation-based solvation models,
Biophys. Chem. **257**, 106258-1–15 (2020);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/bpc-2020-257-106258.pdf>
with Supplementary Data online.

[251] R. Tripathi, H. Forbert, and D. Marx,
Settling the Long-Standing Debate on the Proton Storage Site of the Prototype Light-Driven Proton Pump Bacteriorhodopsin,
J. Phys. Chem. B **123**, 9598–9608 (2019);

Anonymous ftp: <outgoing/dominik_marx/PAPERS/jpcb-2019-123-9598.pdf>
with 23 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jpcb-2019-123-9598-si.pdf>

[250] C. Schran and D. Marx,
Quantum nature of the hydrogen bond from ambient conditions down to ultra-low temperatures,
Phys. Chem. Chem. Phys. **21**, 24967–24975 (2019).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2019-21-24967.pdf>

[249] H. Vondracek, S. Imoto, L. Knake, G. Schwaab, D. Marx, and M. Havenith,
Hydrogen-Bonding in Liquid Water at Multikilobar Pressures,
J. Phys. Chem. B **123**, 7748–7753 (2019);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jcpb-2019-123-7748.pdf>
with 23 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jcpb-2019-123-7748-si.pdf>

[248] C. Hölzl, P. Kibies, S. Imoto, J. Noetzel, M. Knierbein, P. Salmen, M. Paulus, J. Nase, C. Held, G. Sadowski, D. Marx, S. M. Kast, and D. Horinek,
Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description,
Biophys. Chem. **254**, 106260 (2019);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/bpc-2019-254-106260.pdf>
with 17 pages of Supplementary Data.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/bpc-2019-254-106260-si.pdf>

[247] F. Uhl and D. Marx,
Quantum Microsolvation of Protonated Methane with ^{4}He: Large–Amplitude Motion Heavily Influences Bosonic Exchange,
Phys. Rev. Lett. **123**, 123002-1–6 (2019);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL-2019-123-123002.pdf>
with 10 pages of Supplemental Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL-2019-123-123002-SI.pdf>

[246] M. F. Pill, A. L. L. East, D. Marx, M. K. Beyer, and H. Clausen–Schaumann,
Mechanical Activation Drastically Accelerates Amide Bond Hydrolysis, Matching Enzyme Activity,
Angew. Chem. Int. Ed. **58**, 9787–9790 (2019);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-2019-58-9787.pdf>
with 16 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-2019-58-9787-si.pdf>

[245] D. Mani, R. Perez de Tudela, R. Schwan, N. Pal, S. Körning, H. Forbert, B. Redlich, A. F. G. van der Meer, G. Schwaab, D. Marx, and M. Havenith,
Acid solvation versus dissociation at "stardust conditions": Reaction sequence matters,
Sci. Adv. **5**, aav8179-1–7 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/eaav8179.pdf>`
with 39 pages of Supplementary Materials.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/eaav8179-si.pdf>`

[244] N. Kumar and and D. Marx,
How do ribozymes accommodate additional water molecules upon hydrostatic compression deep into the kilobar pressure regime?
Biophys. Chem. **252**, 106192-1–9 (2019).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/biophyschem-2019-252-106192.pdf>`

[243] S. Amirjalayer, H. Fuchs, and D. Marx,
Understanding the Mechanocatalytic Conversion of Biomass: A Low-Energy One-Step Reaction Mechanism by Applying Mechanical Force,
Angew. Chem. Int. Ed. **58**, 5232–5235 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2019-58-5232.pdf>`
with 3 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2019-58-5232-si.pdf>`

[242] P. K. Gupta, A. Esser, H. Forbert, and D. Marx,
Toward Theoretical Terahertz Spectroscopy of Glassy Aqueous Solutions: Partially Frozen Solute-Solvent Couplings of Glycine in Water,
Phys. Chem. Chem. Phys. **21**, 4975–4987 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2019-21-4975.pdf>`
with 8 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2019-21-4975-si.pdf>`

[241] S. Yoo, N. Siemer, M. Todorova, D. Marx, and J. Neugebauer,
Deciphering Charge Transfer and Electronic Polarization Effects at Gold Nanocatalysts on Reduced Titania Support,
J. Phys. Chem. C **123**, 5495–5506 (2019).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcc-2019-123-5495.pdf>`

[240] J. Daru, P. K. Gupta, and D. Marx,
Restricting Solvation to Two Dimensions: Soft-Landing of Microsolvated Ions on Inert Surfaces,
J. Phys. Chem. Lett. **10**, 831–835 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-831.pdf>`
with 29 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-831-si.pdf>`

[239] S. Imoto and D. Marx,
Pressure response of the THz spectrum of bulk liquid water revealed by intermolecular instantaneous normal mode analysis,
J. Chem. Phys. **150**, 084502-1–28 (2019).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2019-150-084502.pdf>`

[238] M. E. Zoloff Michoff, J. Ribas–Arino, and D. Marx,
Selective Nanomechanics of Aromatic versus Aliphatic Thiolates on Gold Surfaces,
Phys. Rev. Lett. **122**, 086801-1–6 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2019-122-086801.pdf>`
with 42 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-2019-122-086801-SI.pdf>`

[237] P. K. Gupta, P. Schienbein, J. Daru, and D. Marx,
Terahertz Spectra of Microsolvated Ions: Do they Reveal Bulk Solvation Properties?
J. Phys. Chem. Lett. **10**, 393–398 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-393.pdf>`
with 24 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-393-si.pdf>`

[236] S. Ruiz–Barragan, D. Munoz–Santiburcio, and D. Marx,
Nanoconfined Water within Graphene Slit Pores Adopts Distinct Confinement–Dependent Regimes,
J. Phys. Chem. Lett. **10**, 329–334 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-329.pdf>`
with 6 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2019-10-329-si.pdf>`

[235] R. Tripathi, J. Noetzel, and D. Marx,
Exposing catalytic versatility of GTPases: taking reaction detours in mutants of hGBP1 enzyme without additional energetic cost,
Phys. Chem. Chem. Phys. **21**, 859–867 (2019);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2019-21-859.pdf>`
with 12 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2019-21-859-si.pdf>`

[234] N. Siemer, A. Lüken, M. Zalibera, J. Frenzel, D. Munoz-Santiburcio, A. Savitsky, W. Lubitz, M. Muhler, D. Marx, and J. Strunk,
Atomic–Scale Explanation of O_2 activation at the Au–TiO_2 Interface,
J. Am. Chem. Soc. **140**, 18082–18092 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jacs-2018-140-18082.pdf>`

with 25 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jacs-2018-140-18082-si.pdf>

[233] F. Uhl and D. Marx,
Helium Tagging of Protonated Methane in Messenger Spectroscopy: Does it Interfere with the Fluxionality of CH_5^+?,
Angew. Chem. Int. Ed. **57**, 14792–14795 (2018).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-2018-57-14792.pdf>

[232] C. Schran, F. Brieuc, and D. Marx,
Converged Colored Noise Path Integral Molecular Dynamics Study of the Zundel Cation down to Ultralow Temperatures at Coupled Cluster Accuracy,
J. Chem. Theory Comput. **14**, 5068–5078 (2018);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jctc-8b00705.pdf>
with 8 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jctc-8b00705-si.pdf>

[231] N. Kumar and and D. Marx,
Mechanistic role of nucleobases in self-cleavage catalysis of hairpin ribozyme at ambient versus high-pressure conditions,
Phys. Chem. Chem. Phys. **20**, 20886–20898 (2018);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2018-20-20886.pdf>
with 9 pages of Electronic Supplementary Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2018-20-20886-si.pdf>

[230] P. Schienbein and D. Marx,
Investigation concerning the uniqueness of separatrix lines separating liquidlike from gaslike regimes deep in the supercritical phase of water with a focus on Widom line concepts,
Phys. Rev. E **98**, 022104-1–11 (2018).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRE-98-022104-2018.pdf>

[229] M. Wollenhaupt, C. Schran, M. Krupicka, and D. Marx,
Force-Induced Catastrophes on Energy Landscapes: Mechanochemical Manipulation of Downhill and Uphill Bifurcations Explains the Ring-Opening Selectivity of Cyclopropanes,
ChemPhysChem **19**, 837–847 (2018);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2018-19-837.pdf>
with 20 pages of Supporting Information;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2018-19-837-SI.pdf>

[228] P. Schienbein and D. Marx,
Liquid-Vapor Phase Diagram of RPBE-D3 Water: Electronic Properties along the Coexistence Curve and in the Supercritical Phase,

J. Phys. Chem. B **122**, 3318–3329 (2018);
part of the "Benjamin Widom Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcb-2018-122-3318.pdf>`

[227] D. Munoz-Santiburcio, M. Farnesi Camellone, and D. Marx,
Solvation-Induced Changes in the Mechanism of Alcohol Oxidation at Gold/Titania Nanocatalysts in the Aqueous Phase versus Gas Phase,
Angew. Chem. Int. Ed. **57**, 3327–3331 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2018-57-3327.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2018-57-3327-all.pdf>`
with 9 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2018-57-3327-si.pdf>`
see also *Cover Picture*;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2018-57-3327-cover.pdf>`

[226] C. Schran, F. Uhl, J. Behler, and D. Marx,
High-dimensional neural network potentials for solvation: The case of protonated water clusters in helium,
J. Chem. Phys. **148**, 102310-1–10 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-148-102310-2018.pdf>`
with 21 pages of Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-148-102310-2018-SI.pdf>`

[225] S. Imoto, H. Forbert, and D. Marx,
Aqueous TMAO solutions as seen by theoretical THz spectroscopy: hydrophilic versus *hydrophobic water,*
Phys. Chem. Chem. Phys. **20**, 6146–6158 (2018).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2018-20-6146.pdf>`

[224] D. Marx and M. I. Menendez,
Torquoselective Mechanochemical Activation of the Staudinger Reaction To Form β–Lactams,
J. Org. Chem. (Note) **83**, 2438–2441 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/joc-7b03036.pdf>`
with 23 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/joc-7b03036-si.pdf>`

[223] A. Esser, H. Forbert, F. Sebastiani, G. Schwaab, M. Havenith, and D. Marx,
Hydrophilic Solvation Dominates the THz Fingerprint of Amino Acids in Water,
J. Phys. Chem. B **122**, 1453–1459 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcb-2018-122-1453.pdf>`
with 71 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcb-2018-122-1453-si.pdf>`

[222] A. Esser, H. Forbert, and D. Marx,
Tagging effects on the mid-infrared spectrum of microsolvated protonated methane,
Chem. Sci. **9**, 1560–1573 (2018);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-2018-9-1560.pdf>`
with 15 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-2018-9-1560-si.pdf>`

[221] R. Perez de Tudela and D. Marx,
Acid Dissociation in HCl-Water Clusters is Temperature Dependent and Cannot be Detected Based on Dipole Moments,
Phys. Rev. Lett. **119**, 223001-1–6 (2017);
Publisher's Note: Phys. Rev. Lett. **119**, 259901-1 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-119-223001-2017.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-119-259901-2017-Note.pdf>`
with 7 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-119-223001-2017-SI.pdf>`

[220] D. Munoz-Santiburcio and D. Marx,
Nanoconfinement in Slit Pores Enhances Water Self–Dissociation,
Phys. Rev. Lett. **119**, 056002-1–6 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-119-056002.pdf>`
with 10 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-119-056002-SI.pdf>`

[219] J. Frenzel, B. Meyer, and D. Marx,
Bicanonical ab Initio Molecular Dynamics for Open Systems,
J. Chem. Theory Comput. **13**, 3455–3469 (2017).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/acs.jctc.7b00263.pdf>`

[218] M. Krupicka, P. Dopieralski, and D. Marx,
Unclicking the Click: Metal–Assisted Mechanochemical Cycloreversion of Triazoles is Possible,
Angew. Chem. Int. Ed. **56**, 7745–7749 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2017-56-7745.pdf>`
with 53 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-2017-56-7745-si.pdf>`

[217] P. Schienbein, G. Schwaab, H. Forbert, M. Havenith, and D. Marx,
Correlations in the Solute–Solvent Dynamics Reach Beyond the First Hydration Shell of Ions,
J. Phys. Chem. Lett. **8**, 2373–2380 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2017-8-2373.pdf>`
with 38 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2017-8-2373-si.pdf>`

[216] D. Munoz–Santiburcio and D. Marx,
Chemistry in nanoconfined water,
Chem. Sci. **8**, 3444–3452 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-2017-8-3444.pdf>`
with 37 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-2017-8-3444-si.pdf>`

[215] C. Schuabb, N. Kumar, S. Pataraia, D. Marx, and R. Winter,
Pressure modulates the self-cleavage step of the hairpin ribozyme,
Nat. Commun. **8**, 14661–1-10 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ncomms14661.pdf>`
with 8 pages of Supplementary Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ncomms14661-si.pdf>`

[214] D. Kuchenbecker, F. Uhl, H. Forbert, G. Jansen, and D. Marx,
Constructing accurate interaction potentials to describe the microsolvation of protonated methane by helium atoms,
Phys. Chem. Chem. Phys. **19**, 8307–8321 (2017).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2017-19-8307.pdf>`

[213] A. Esser, S. Belsare, D. Marx, and T. Head-Gordon,
Mode specific THz spectra of solvated amino acids using the AMOEBA polarizable force field,
Phys. Chem. Chem. Phys. **19**, 5579–5590 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c6cp07388c1.pdf>`
with 52 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c6cp07388c1-SI.pdf>`

[212] T. Zelleke and D. Marx,
Free-Energy Landscape and Proton Transfer Pathways in Oxidative Deamination by Methylamine Dehydrogenase,
ChemPhysChem **18**, 208–222 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2017-18-208.pdf>`
with 14 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2017-18-208-SI.pdf>`

[211] C. Drechsel–Grau and D. Marx,
Collective proton transfer in ordinary ice: local environments, temperature dependence and deuteration effects,
Phys. Chem. Chem. Phys. **19**, 2623–2635 (2017);
see also *Cover Picture* on Issue 4 of Volume 19 (28 January 2017);
highlighted by the PCCP Editors as a "HOT manuscript in 2017".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2017-19-2623.pdf>`

[210] P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, and D. Marx,
Unexpected mechanochemical complexity in the mechanistic scenarios of disulfide bond reduction in alkaline solution,
Nat. Chem. **9**, 164–170 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/natchem-9-164-2017.pdf>`
with 34 pages of Supplementary Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/natchem-9-164-2017-si.pdf>`

[209] R. Tripathi, R. Glaves, and D. Marx,
The GTPase hGBP1 converts GTP to GMP in two steps via *proton shuttle mechanisms,*
Chem. Sci. **8**, 371–380 (2017);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-8-371-2017.pdf>`
with 28 pages of Electronic Supplementary Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemsci-8-371-2017-SI.pdf>`

[208] R. Perez de Tudela and D. Marx,
Water-Induced Zwitterionization of Glycine: Stabilization Mechanism and Spectral Signatures,
J. Phys. Chem. Lett. **7**, 5137–5142 (2016);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2016-7-5137.pdf>`
with 150 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2016-7-5137-si.pdf>`

[207] D. Munoz–Santiburcio and D. Marx,
On the complex structural diffusion of proton holes in nanoconfined alkaline solutions within slit pores,
Nat. Commun. **7**, 12625–1-9 (2016).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/natcommun-7-12625-2016.pdf>`
`<outgoing/dominik_marx/PAPERS/natcommun-7-12625-2016-reviews.pdf>`

[206] F. Uhl, D. Marx, and M. Ceriotti,
Accelerated path integral methods for atomistic simulations at ultra-low temperatures,
J. Chem. Phys. **145**, 054101–1-9 (2016).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-145-054101-2016.pdf>`

[205] S. Imoto, P. Kibies, C. Rosin, R. Winter, S. M. Kast, and D. Marx,
Toward Extreme Biophysics: Deciphering the Infrared Response of Biomolecular Solutions at High Pressures,
Angew. Chem. Int. Ed. **55**, 9534–9538 (2016);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201602757.pdf>`
with 9 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201602757-SI.pdf>`

[204] C. Hölzl, P. Kibies, S. Imoto, R. Frach, S. Suladze, R. Winter, D. Marx, D. Horinek, and S. M. Kast,
Design principles for high-pressure force fields: Aqueous TMAO solutions from ambient to kilobar pressures,
J. Chem. Phys. **144**, 144104–1-16 (2016);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-144-144104-2016.pdf>`
with 4 pages of Supplementary Material (pdf) and optimized structures (txt);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-144-144104-2016-SI.pdf>`
`<outgoing/dominik_marx/PAPERS/JCP-144-144104-2016-SI2.txt>`
see also *Cover Picture* on Issue 14 of Volume 144 (14 April 2016).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-144-144104-2016-COV.pdf>`
elected by JCP as 2016 Editors' Choice Article being one of "the most innovative and influential articles of 2016".

[203] P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, and D. Marx,
Force–Induced Reversal of β–Eliminations: Stressed Disulfide Bonds in Alkaline Solution,
Angew. Chem. Int. Ed. **55**, 1304–1308 (2016);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201508005.pdf>`
with 12 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201508005-SI.pdf>`

[202] M. Smiechowski, C. Schran, H. Forbert, and D. Marx,
Correlated Particle Motion and THz Spectral Response of Supercritical Water,
Phys. Rev. Lett. **116**, 027801–1-6 (2016);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-116-027801.pdf>`
with 23 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-116-027801-SI.pdf>`

[201] S. D. Ivanov, I. M. Grant, and D. Marx,
Quantum free energy landscapes from ab initio *path integral metadynamics: Double proton transfer in the formic acid dimer is concerted but not correlated,*
J. Chem. Phys. **143**, 124304–1-9 (2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-143-124304-2015.pdf>`

[200] S. Imoto, H. Forbert, and D. Marx,
Water structure and solvation of osmolytes at high hydrostatic pressure: pure water and TMAO solutions at 10 kbar versus *1 bar,*
Phys. Chem. Chem. Phys. **17**, 24224–24237 (2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2015-17-24224.pdf>`

[199] P. Seema, J. Behler, and D. Marx,
Peeling by Nanomechanical Forces: A Route to Selective Creation of Surface Structures,

Phys. Rev. Lett. **115**, 036102–1-5 (2015).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL-115-036102.pdf>

[198] M. Böckmann, N. L. Doltsinis, and D. Marx,
Adaptive Switching of Interaction Potentials in the Time Domain: An Extended Lagrangian Approach Tailored to Transmute Force Field to QM/MM Simulations and Back,
J. Chem. Theory Comput. **11**, 2429–2439 (2015).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCTC-2015-11-2429.pdf>

[197] L. Martinez–Suarez, N. Siemer, J. Frenzel, and D. Marx,
Reaction Network of Methanol Synthesis over Cu/ZnO Nanocatalysts,
ACS Catal. **5**, 4201–4218 (2015);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/AcsCatal-2015-5-4201.pdf>
with 11 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/AcsCatal-2015-5-4201-SI.pdf>

[196] M. Wollenhaupt, M. Krupicka, and D. Marx,
Should the Woodward-Hoffmann Rules be Applied to Mechanochemical Reactions?,
ChemPhysChem (Communication) **16**, 1593–1597 (2015);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2015-16-1593.pdf>
with 10 pages of Supporting Information;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2015-16-1593-SI.pdf>
see also *Cover Picture* of Issue 16(8) and *Cover Profile* on p. 1565.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2015-16-1593-Cover1.pdf>
<outgoing/dominik_marx/PAPERS/CPC-2015-16-1593-Cover2.pdf>

[195] M. Smiechowski, J. Sun, H. Forbert, and D. Marx,
Solvation shell resolved THz spectra of simple aqua ions – distinct distance- and frequency-dependent contributions of solvation shells,
Phys. Chem. Chem. Phys. **17**, 8323–8329 (2015);
part of the PCCP Themed Issue "Solvation Science";
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2015-17-8323.pdf>
with 18 pages of Electronic Supplementary Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-2015-17-8323-si.pdf>

[194] M. Krupicka and D. Marx,
Disfavoring Mechanochemical Reactions by Stress-Induced Steric Hindrance,
J. Chem. Theory Comput. (Letter) **11**, 841–846 (2015);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ct501058a.pdf>
with 34 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ct501058a-si.pdf>

[193] Md. E. Ali, V. Staemmler, and D. Marx,
Magnetostructural dynamics of Rieske versus *ferredoxin iron-sulfur cofactors,*
Phys. Chem. Chem. Phys. **17**, 6289–6296 (2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2015-17-6289.pdf>`

[192] M. E. Zoloff Michoff, J. Ribas–Arino, and D. Marx,
Nanomechanics of Bidentate Thiolate Ligands on Gold Surfaces,
Phys. Rev. Lett. **114**, 075501–1-5 (2015);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-114-075501.pdf>`
with 38 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-114-075501-SI.pdf>`

[191] Md. E. Ali, N. N. Nair, M. Retegan, F. Neese, V. Staemmler, and D. Marx,
The iron-sulfur core in Rieske proteins is not symmetric,
J. Biol. Inorg. Chem. **19**, 1287–1293 (2014).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JBIC-2014-19-1287.pdf>`

[190] L. Martinez–Suarez, J. Frenzel, and D. Marx,
Cu/ZnO nanocatalysts in response to environmental conditions: surface morphology, electronic structure, redox state and CO_2 activation,
Phys. Chem. Chem. Phys. **16**, 26119–26136 (2014);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PCCP-2014-16-26119.pdf>`
with 21 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PCCP-2014-16-26119-SI.pdf>`

[189] P. Anjukandi, P. Dopieralski, J. Ribas–Arino, and D. Marx,
The Effect of Tensile Stress on the Conformational Free Energy Landscape of Disulfide Bonds,
PLOS ONE **9**, e108812–1-7 (2014);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PONE-9-e108812-2014.pdf>`
with 15 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PONE-9-e108812-2014-SI.pdf>`

[188] C. Drechsel–Grau and D. Marx,
Exceptional Isotopic-Substitution Effect: Breakdown of Collective Proton Tunneling in Hexagonal Ice due to Partial Deuteration,
Angew. Chem. Int. Ed. **53**, 10937–10940 (2014);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201405989.pdf>`
with 2 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-201405989-si.pdf>`
Exceptional Isotopic-Substitution Effect: Breakdown of Collective Proton Tunneling in Hexagonal Ice due to Partial Deuteration,
Angew. Chem. **126**, 11117–11120 (2014);

Anonymous ftp: <outgoing/dominik_marx/PAPERS/ange-201405989.pdf>
Featured as a *"Very Important Paper" (VIP).*

[187] J. Frenzel and D. Marx,
Methanol synthesis on ZnO($000\bar{1}$*). IV. Reaction mechanisms and electronic structure,*
J. Chem. Phys. **141**, 124710–1-20 (2014).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-141-124710-2014.pdf>

[186] F. Uhl, L. Walewski, H. Forbert, and D. Marx,
Adding flexibility to the "particles-on-a-sphere" model for large-amplitude motion: POSflex force field for protonated methane,
J. Chem. Phys. **141**, 104110–1-12 (2014);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-141-104110-2014.pdf>
with 8 pages of Supporting Information including 6 Videos.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-141-104110-2014-SI.pdf>

[185] M. Farnesi Camellone and D. Marx,
Nature and Role of Activated Molecular Oxygen Species at the Gold/Titania Interface in the Selective Oxidation of Alcohols,
J. Phys. Chem. C **118**, 20989–21000 (2014).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jp5060233.pdf>

[184] J. Sun, G. Niehues, H. Forbert, D. Decka, G. Schwaab, D. Marx, and M. Havenith,
Understanding THz Spectra of Aqueous Solutions: Glycine in Light and Heavy Water,
J. Am. Chem. Soc. **136**, 5031–5038 (2014);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja4129857.pdf>
with 28 pages of Supporting Information including 16 Videos.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja4129857-si.pdf>

[183] L. Walewski, H. Forbert, and D. Marx,
Solvation of molecules in superfluid helium enhances the "interaction induced localization" effect,
J. Chem. Phys. **140**, 144305–1-14 (2014).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-140-144305-2014.pdf>

[182] C. Drechsel–Grau and D. Marx,
Quantum Simulation of Collective Proton Tunneling in Hexagonal Ice Crystals,
Phys. Rev. Lett. **112**, 148302–1-5 (2014);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL-112-148302.pdf>
with 21 pages of Supplemental Material and additional 3 Videos.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL-112-148302-SI.pdf>
<outgoing/dominik_marx/PAPERS/supplemental-video-1-Drechsel-Grau-Marx.zip>

`<outgoing/dominik_marx/PAPERS/supplemental-video-2-Drechsel-Grau-Marx.zip>`
`<outgoing/dominik_marx/PAPERS/supplemental-video-3-Drechsel-Grau-Marx.zip>`

[181] M. Krupicka, W. Sander, and D. Marx,
Mechanical Manipulation of Chemical Reactions: Reactivity Switching of Bergman Cyclizations,
J. Phys. Chem. Lett. **5**, 905–909 (2014);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jz402644e.pdf>`
with 33 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jz402644e-si.pdf>`
see also coverage in the media:
D. Bradley: *Mechanical stress pulls cyclisation into shape,* Chemistry World, 3 March 2014.

[180] L. Walewski, H. Forbert, and D. Marx,
Reactive path integral quantum simulations of molecules solvated in superfluid helium,
Comput. Phys. Commun. **185**, 884–899 (2014).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/COMPUTPC-185-884-2014.pdf>`

[179] M. Letzner, S. Gruen, D. Habig, K. Hanke, T. Endres, P. Nieto, G. Schwaab, L. Walewski, M. Wollenhaupt, H. Forbert, D. Marx, and M. Havenith,
High resolution spectroscopy of HCl-water clusters: IR bands of undissociated and dissociated clusters revisited,
J. Chem. Phys. **139**, 154304–1-11 (2013).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-139-154304-2013.pdf>`

[178] L. Walewski, H. Forbert, and D. Marx,
Interaction-induced localization of protons in hydrogen bonds at superfluid helium temperatures,
Mol. Phys. **111**, 2555–2569 (2013);
part of the "Werner Kutzelnigg Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/MolPhys-111-2555-2013.pdf>`

[177] P. Seema, J. Behler, and D. Marx,
Force–induced mechanical response of molecule–metal interfaces: molecular nanomechanics of propanethiolate self–assembled monolayers on Au(111),
Phys. Chem. Chem. Phys. **15**, 16001–16011 (2013).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-15-16001-2013.pdf>`

[176] M. Böckmann, S. Braun, N. L. Doltsinis, and D. Marx,
Mimicking photoisomerisation of azo-materials by a force field switch derived from nonadiabatic ab initio *simulations: Application to photoswitchable helical foldamers in solution,*

J. Chem. Phys. **139**, 084108–1-10 (2013);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-139-084108-2013.pdf>
with 10 pages of Supporting Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-139-084108-2013-SI.pdf>

[175] D. Munoz–Santiburcio, C. Wittekindt and D. Marx,
Nanoconfinement effects on hydrated excess protons in layered materials,
Nat. Commun. **4**, 2349–1-5 (2013).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/natcommun-4-2349-2013.pdf>

[174] J. Kiss, J. Frenzel, B. Meyer, and D. Marx,
Methanol synthesis on ZnO($000\bar{1}$*). II. Structure, energetics, and vibrational signature of reaction intermediates,*
J. Chem. Phys. **139**, 044705–1-17 (2013);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-139-044705-2013.pdf>
with 13 pages of Supporting Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-139-044705-2013-SI.pdf>

[173] P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, J. Kiss, and D. Marx,
The Janus-faced role of external forces in mechanochemical disulfide bond cleavage,
Nat. Chem. **5**, 685–691 (2013);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/natchem-5-685-2013.pdf>
with 30 pages of Supplementary Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/natchem-5-685-2013-si.pdf>

[172] M. Smiechowski, H. Forbert, and D. Marx,
Communication: Spatial decomposition and assignment of infrared spectra of simple ions in water from mid-infrared to THz frequencies: $Li^+(aq)$ *and* $F^-(aq)$*,*
J. Chem. Phys. **139**, 014506–1-15 (2013).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-139-014506-2013.pdf>

[171] M. Farnesi Camellone, J. Zhao, L. Jin, Y. Wang, M. Muhler, and D. Marx,
Molecular Understanding of Reactivity and Selectivity for Methanol Oxidation at the Au/TiO_2 *Interface,*
Angew. Chem. Int. Ed. **52**, 5780–5784 (2013);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-52-5780-2013.pdf>
with 20 pages of Supporting Information;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-52-5780-2013-SI.pdf>
Molecular Understanding of Reactivity and Selectivity for Methanol Oxidation at the Au/TiO_2 *Interface,*
Angew. Chem. **125**, 5892–5896 (2013).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ange-125-5892-2013.pdf>

[170] L. Walewski, H. Forbert, and D. Marx,
Revealing the Subtle Interplay of Thermal and Quantum Fluctuation Effects on Contact Ion Pairing in Microsolvated HCl,
ChemPhysChem **14**, 817–826 (2013);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2013-14-817.pdf>`
with 9 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2013-14-817-SI.pdf>`

[169] A. Witt, S. D. Ivanov, and D. Marx,
Microsolvation–Induced Quantum Localization in Protonated Methane,
Phys. Rev. Lett. **110**, 083003–1-5 (2013);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-110-083003.pdf>`
with 9 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-110-083003-SI.pdf>`

[168] L. Martinez–Suarez, J. Frenzel, D. Marx, and B. Meyer,
Tuning the Reactivity of a Cu/ZnO Nanocatalyst via Gas Phase Pressure,
Phys. Rev. Lett. **110**, 086108–1-5 (2013);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-110-086108.pdf>`
with 9 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-110-086108-SI.pdf>`

[167] P. Seema, J. Behler, and D. Marx,
Adsorption of Methanethiolate and Atomic Sulfur at the Cu(111) Surface: A Computational Study,
J. Phys. Chem. C **117**, 337–348 (2013).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcc-2013-117-337.pdf>`

[166] M. Farnesi Camellone and D. Marx,
On the Impact of Solvation on a Au/TiO_2 Nanocatalyst in Contact with Water,
J. Phys. Chem. Lett. **4**, 514–518 (2013);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jz301891v.pdf>`
with 9 pages of Supplemental Material.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jz301891v-si.pdf>`

[165] C. Wittekindt and D. Marx,
Water confined between sheets of mackinawite FeS minerals,
J. Chem. Phys. **137**, 054710–1-8 (2012).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-137-054710-2012.pdf>`

[164] M. Böckmann, N. L. Doltsinis, and D. Marx,
Enhanced photoswitching of bridged azobenzene studied by nonadiabatic ab initio simulation,

J. Chem. Phys. **137**, 22A505–1-10 (2012).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-137-22A505-2012.pdf>

[163] M. Heyden, J. Sun, H. Forbert, G. Mathias, M. Havenith, and 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);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jz300748s.pdf>
with 15 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jz300748s-si.pdf>

[162] Md. E. Ali, N. N. Nair, V. Staemmler, and D. Marx,
Constrained spin-density dynamics of an iron-sulfur complex: Ferredoxin cofactor,
J. Chem. Phys. **136**, 224101–1-8 (2012).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP-136-224101-2012.pdf>

[161] R. Glaves, G. Mathias, and D. Marx,
Mechanistic Insights into the Hydrolysis of a Nucleoside Triphosphate Model in Neutral and Acidic Solution,
J. Am. Chem. Soc. **134**, 6995–7000 (2012);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja2101533.pdf>
with 18 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja2101533-si.pdf>

[160] J. Lessing, S. Roy, M. Reppert, M. Baer, D. Marx, T. L. C. Jansen, J. Knoester, and A. Tokmakoff,
Identifying Residual Structure in Intrinsically Disordered Systems: A 2D IR Spectroscopic Study of the GVGXPGVG Peptide,
J. Am. Chem. Soc. (Communication) **134**, 5032–5035 (2012);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja2114135.pdf>
with 10 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja2114135-si.pdf>

[159] S. Braun, M. Böckmann, and D. Marx,
Unfolding a Photoswitchable Azo-Foldamer Reveals a Non-Covalent Reaction Mechanism,
ChemPhysChem (Communication) **13**, 1140–1443 (2012).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-13-1440-2012.pdf>

[158] G. Mathias, S. D. Ivanov, A. Witt, M. D. Baer, and D. Marx,
Infrared Spectroscopy of Fluxional Molecules from (ab Initio) Molecular Dynamics: Resolving Large-Amplitude Motion, Multiple Conformations, and Permutational Symmetries,

J. Chem. Theory Comput. **8**, 224–234 (2012).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ct2006665.pdf>`

[157] M. Farnesi Camellone and D. Marx,
Solvation of Au^+ versus Au^0 in aqueous solution: electronic structure governs solvation shell patterns,
Phys. Chem. Chem. Phys. **14**, 937–944 (2012).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2012-14-937.pdf>`

[156] L. Walewski, H. Forbert, and D. Marx,
Quantum Induced Bond Centering in Microsolvated HCl: Solvent Separated versus Contact Ion Pairs,
J. Phys. Chem. Lett. **2**, 3069–3074 (2011).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2011-2-3069.pdf>`

[155] A. D. Boese, H. Forbert, M. Masia, A. Tekin, D. Marx, and G. Jansen,
Constructing simple yet accurate potentials for describing the solvation of HCl/water clusters in bulk helium and nanodroplets,
Phys. Chem. Chem. Phys. **13**, 14550–14564 (2011);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c1cp20991d.pdf>`
with 10 pages of Electronic Supplementary Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c1cp20991d-si.pdf>`

[154] A. Witt, S. D. Ivanov, G. Mathias, and D. Marx,
Quantum Molecular Dynamics Calculations of Ultrafast Timescales and Infrared Spectra of Protonated Methane: Quantifying Isotope-Specific Lifetimes,
J. Phys. Chem. Lett. **2**, 1377–1381 (2011).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcl-2-1377-2011.pdf>`

[153] P. Dopieralski, J. Ribas–Arino, and D. Marx,
Force–Transformed Free–Energy Surfaces and Trajectory–Shooting Simulations Reveal the Mechano–Stereochemistry of Cyclopropane Ring–Opening Reactions,
Angew. Chem. Int. Ed. **50**, 7105–7108 (2011);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-50-7105-2011.pdf>`
with 15 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/anie-50-7105-2011-SI.pdf>`
Force–Transformed Free–Energy Surfaces and Trajectory–Shooting Simulations Reveal the Mechano–Stereochemistry of Cyclopropane Ring–Opening Reactions,
Angew. Chem. **123**, 7243–7246 (2011).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ange-123-7243-2011.pdf>`

[152] M. Farnesi Camellone, P. M. Kowalski, and D. Marx,
Ideal, defective, and gold-promoted rutile TiO_2(110) surfaces interacting with CO, H_2, and H_2O: Structures, energies, thermodynamics, and dynamics from PBE+U,

Phys. Rev. B **84**, 035413–1-18 (2011).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prb-84-035413-2011.pdf>`

[151] M. Baer, D. Marx, and G. Mathias,
Assigning Predissociation Infrared Spectra of Microsolvated Hydronium Cations $H_3O^+\cdot(H_2)_n$ ($n = 0, 1, 2, 3$) by Ab Initio Molecular Dynamics,
ChemPhysChem **12**, 1906–1915 (2011);
part of the "Karl Kleinermanns Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cpc-12-1906-2011.pdf>`

[150] R. Pollet, N. N. Nair, and D. Marx,
Water Exchange of a ProHance MRI Contrast Agent: Isomer–Dependent Free–Energy Landscapes and Mechanisms,
Inorg. Chem. **50**, 4791–4797 (2011);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ic102403r.pdf>`
with 2 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ic102403r-si.pdf>`

[149] P. Dopieralski, P. Anjukandi, M. Rückert, M. Shiga, J. Ribas–Arino, and D. Marx,
On the role of polymer chains in transducing external mechanical forces to benzocyclobutene mechanophores,
J. Mater. Chem. **21**, 8309–8316 (2011).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jmc-2011-21-8309.pdf>`

[148] E. Schreiner, N. N. Nair, C. Wittekindt, and D. Marx,
Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions and Pyrite Mineral Surfaces on Formation and Hydrolysis of Peptides,
J. Am. Chem. Soc. **133**, 8216–8226 (2011);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja111503z.pdf>`
with 6 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja111503z-si.pdf>`

[147] H. Forbert, M. Masia, A. Kaczmarek–Kedziera, N. N. Nair, and D. Marx,
Aggregation–Induced Chemical Reactions: Acid Dissociation in Growing Water Clusters,
J. Am. Chem. Soc. **133**, 4062–4072 (2011);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja1099209.pdf>`
with 2 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja1099209-si.pdf>`

[146] J. Kiss, J. Frenzel, N. N. Nair, B. Meyer, and D. Marx,
Methanol synthesis on ZnO($000\bar{1}$). III. Free energy landscapes, reaction pathways, and mechanistic insights,
J. Chem. Phys. **134**, 064710–1-14 (2011);

Anonymous ftp: <outgoing/dominik_marx/PAPERS/jcp134-11-064710.pdf>
with 4 pages of Supporting Material.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jcp134-11-064710-si.pdf>

[145] R. Turanský, M. Konôpka, N. L. Doltsinis, I. Štich, and D. Marx,
Switching of functionalized azobenzene suspended between gold tips by mechanochemical, photochemical, and opto–mechanical means,
Phys. Chem. Chem. Phys. **12**, 13922–13932 (2010);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-C0CP00588F.pdf>
see also *Cover Picture* on p. 13853.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-C0CP00588F-cover.pdf>

[144] M. Baer, D. Marx, and G. Mathias,
Theoretical Messenger Spectroscopy of Microsolvated Hydronium and Zundel Cations,
Angew. Chem. Int. Ed. **49**, 7346–7349 (2010);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-2010-49-7346.pdf>
with 5 pages of Supporting Information;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/anie-201001672-si.pdf>
Theoretische Botenspektroskopie von mikrosolvatisierten Hydronium– und Zundel–Kationen,
Angew. Chem. **122**, 7504–7507 (2010);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ange-2010-122-7504.pdf>
Featured as a *"Very Important Paper" (VIP)* (... "according to the evaluation of two referees. Less than 5 % of our manuscripts receive such a positive evaluation").

[143] S. A. Fiethen, V. Staemmler, N. N. Nair, J. Ribas–Arino, E. Schreiner, and D. Marx,
Revealing the Magnetostructural Dynamics of [2Fe–2S] Ferredoxins from Reduced–Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations,
J. Phys. Chem. B **114**, 11612–11619 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jp1014912.pdf>

[142] M. E. Tuckerman, A. Chandra, and D. Marx,
A statistical mechanical theory of proton transport kinetics in hydrogen–bonded networks based on population correlation functions with applications to acids and bases,
J. Chem. Phys. **133**, 124108–1-22 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCPSA613312124108.pdf>

[141] P. M. Kowalski, M. Farnesi Camellone, N. N. Nair, B. Meyer, and D. Marx,
Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO_2(110) Surface,
Phys. Rev. Lett. **105**, 146405-1–4 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prl-105-146405.pdf>

[140] J. Sun, D. Bousquet, H. Forbert, and D. Marx,
Glycine in aqueous solution: solvation shells, interfacial water, and vibrational spectroscopy from ab initio *molecular dynamics,*
J. Chem. Phys. **133**, 114508–1-10 (2010).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCPSA613311114508.pdf>`

[139] M. Heyden, J. Sun, S. Funkner, G. Mathias, H. Forbert, M. Havenith, and D. Marx,
Dissecting the THz spectrum of liquid water from first principles via correlations in time and space,
Proc. Natl. Acad. Sci. USA **107**, 12068–12073 (2010).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pnas-0914885107.pdf>`

[138] J. Ribas–Arino, M. Shiga, and D. Marx,
Mechanochemical Transduction of Externally Applied Forces to Mechanophores,
J. Am. Chem. Soc. **132**, 10609–10614 (2010);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja104958e.pdf>`
with 13 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja104958e-si.pdf>`

[137] M. Böckmann, N. L. Doltsinis, and D. Marx,
Unraveling a Chemically Enhanced Photoswitch: Bridged Azobenzene,
Angew. Chem. Int. Ed. **49**, 3382–3384 (2010);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/azo-ANIE-49-3382-2010.pdf>`
Unraveling a Chemically Enhanced Photoswitch: Bridged Azobenzene,
Angew. Chem. **122**, 3454–3456 (2010).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/azo-ANGE-122-3454-2010.pdf>`

[136] S. D. Ivanov, O. Asvany, A. Witt, E. Hugo, G. Mathias, B. Redlich, D. Marx, and S. Schlemmer,
Quantum–induced symmetry breaking explains infrared spectra of CH_5^+ isotopologues,
Nat. Chem. **2**, 298–302 (2010);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/natchem-2010-2-298.pdf>`
with 16 pages of Supplementary Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/natchem-2010-2-298-si.pdf>`
see also coverage in the media:
G. Niedner–Schatteburg: *Brennpunkt: Wählerisches Deuterium*, Physik Journal **9(5)**, 18–19 (2010).

[135] R. Turanský, M. Konôpka, N. L. Doltsinis, I. Štich, and D. Marx,
Optical, Mechanical, and Opto–Mechanical Switching of Anchored Dithioazobenzene Bridges,

ChemPhysChem (Communication) **11**, 345–348 (2010);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2010-11-345.pdf>
see also *Cover Picture* on p. 317.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/CPC-2010-11-345-cov.pdf>

[134] N. N. Nair, J. Ribas–Arino, V. Staemmler, and D. Marx,
Magnetostructural Dynamics from Hubbard–U Corrected Spin–Projection: [2Fe–2S] Complex in Ferredoxin,
J. Chem. Theory Comput. **6**, 569–575 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ct900547w.pdf>

[133] M. Böckmann, N. L. Doltsinis, and D. Marx,
Nonadiabatic Hybrid Quantum and Molecular Mechanic Simulations of Azobenzene Photoswitching in Bulk Liquid Environment,
J. Phys. Chem. A **114**, 745–754 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JPCA-114-745-2010.pdf>

[132] S. D. Ivanov, A. Witt, M. Shiga, and D. Marx,
Communications: On artificial frequency shifts in infrared spectra obtained from centroid molecular dynamics: Quantum liquid water,
J. Chem. Phys. (Communication) **132**, 031101–1-4 (2010).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCPSA61323031101.pdf>

[131] J. Ribas–Arino, M. Shiga, and D. Marx,
Unravelling the Mechanism of Force–Induced Ring–Opening of Benzocyclobutenes,
Chem. Eur. J. (Communication) **15**, 13331–13335 (2009).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/mechano-cej15-13331-2009.pdf>

[130] E. Schreiner, N. N. Nair, and D. Marx,
Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions on Peptide Bond Formation and Peptide Hydrolysis,
J. Am. Chem. Soc. **131**, 13668–13675 (2009);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja9032742.pdf>
with 4 pages of Supporting Information.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja9032742-SI.pdf>

[129] A. Gutberlet, G. Schwaab, Ö. Birer, M. Masia, A. Kaczmarek, H. Forbert, M. Havenith, and D. Marx,
Aggregation–Induced Dissociation of $HCl(H_2O)_4$ Below 1 K: The Smallest Droplet of Acid,
Science **324**, 1545–1548 (2009);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/science-324-1545-2009.pdf>
with 19 pages of Supporting Online Material;
Anonymous ftp: <outgoing/dominik_marx/PAPERS/science-som-324-1545-2009.pdf>

see also corresponding *Perspective* article (Chemistry): T. S. Zwier: *Squeezing the Water Out of HCl(aq)* in Science **324**, 1522–1523 (2009);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/science-324-1522-2009.pdf>`
see also coverage in the media:
Chemistry: The tiniest acid drop, Nature (London) **459**, 1036–1036 (2009);
Formation of the smallest droplet of acid: New reaction mechanism at ultracold temperatures, Chemie.DE Information Service GmbH: www.chemie.de/news/e/102330/ (22.06.2009); *Neuer Reaktionsmechanismus bei ultrakalten Temperaturen*, GIT Labor–Fachzeitschrift **53(8)**, 486 (2009).

[128] A. Witt, S. D. Ivanov, M. Shiga, H. Forbert, and D. Marx,
On the applicability of centroid and ring polymer path integral molecular dynamics for vibrational spectroscopy,
J. Chem. Phys. **130**, 194510–1-15 (2009).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCPSA613019194510.pdf>`

[127] M. Konôpka, R. Turanský, M. Dubecký, D. Marx, and I. Štich,
Molecular Mechanochemistry Understood at the Nanoscale: Thiolate Interfaces and Junctions with Copper Surfaces and Clusters,
J. Phys. Chem. C **113**, 8878–8887 (2009);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jp9017025.pdf>`
with 38 pages of Supporting Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jp9017025-si.pdf>`

[126] J. Ribas–Arino, M. Shiga, and D. Marx,
Understanding Covalent Mechanochemistry,
Angew. Chem. Int. Ed. **48**, 4190–4193 (2009);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-anie-09.pdf>`
with 10 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-anie-09-si.pdf>`
Understanding Covalent Mechanochemistry,
Angew. Chem. **121**, 4254–4257 (2009);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew-09.pdf>`
Featured as a *"Hot Paper"* (... "chosen by the Editors for their importance in a rapidly evolving field of high current interest").
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-anie-09-toc.pdf>`

[125] J. Kiss, A. Witt, B. Meyer, and D. Marx,
Methanol synthesis on ZnO($000\bar{1}$*). I. Hydrogen coverage, charge state of oxygen vacancies, and chemical reactivity,*
J. Chem. Phys. **130**, 184706–1-14 (2009).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp130-09-184706.pdf>`

[124] E. C. Beret, R. R. Pappalardo, D. Marx, and E. Sánchez Marcos,
Characterizing Pt–Derived Anticancer Drugs from First Principles: The Case of Oxaliplatin in Aqueous Solution,
ChemPhysChem **10**, 1044–1052 (2009).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/CPC-2009-10-1044.pdf>`

[123] M. Kunat, F. Traeger, D. Silber, H. Qiu, Y. Wang, A. C. van Veen, Ch. Wöll, P. M. Kowalski, B. Meyer, C. Hättig, and D. Marx,
Formation of weakly bound, ordered adlayers of CO on rutile TiO_2(110): A combined experimental and theoretical study,
J. Chem. Phys. **130**, 144703–1-11 (2009).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp130-09-144703.pdf>`

[122] A. Kaczmarek, M. Shiga, and D. Marx,
Quantum Effects on Vibrational and Electronic Spectra of Hydrazine Studied by "On–the–Fly" ab Initio *Ring Polymer Molecular Dynamics,*
J. Phys. Chem. A **113**, 1985–1994 (2009);
part of the "Max Wolfsberg Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JPCA2009-113-1985.pdf>`

[121] P. M. Kowalski, B. Meyer, and D. Marx,
Composition, structure, and stability of the rutile TiO_2(110) surface: Oxygen depletion, hydroxylation, hydrogen migration and water adsorption,
Phys. Rev. B **79**, 115410–1-16 (2009).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prb79-09-115410.pdf>`

[120] R. Glaves, M. Baer, E. Schreiner, R. Stoll, and D. Marx,
Conformational Dynamics of Minimal Elastin–Like Polypeptides: The Role of Proline Revealed by Molecular Dynamics and Nuclear Magnetic Resonance,
ChemPhysChem **9**, 2759–2765 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ChemPhysChem-2008-9-2759.pdf>`

[119] A. Chaumont, M. Baer, G. Mathias, and D. Marx,
Potential Proton–Release Channels in Bacteriorhodopsin,
ChemPhysChem **9**, 2751–2758 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ChemPhysChem-2008-9-2751.pdf>`

[118] M. Baer, G. Mathias, I–F. W. Kuo, D. J. Tobias, C. J. Mundy, and D. Marx,
Spectral Signatures of the Pentagonal Water Cluster in Bacteriorhodopsin,
ChemPhysChem (Communication) **9**, 2703–2707 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ChemPhysChem-2008-9-2703.pdf>`

[117] E. C. Beret, J. M. Martínez, R. R. Pappalardo, E. Sánchez Marcos, N. L. Doltsinis, and D. Marx,

Explaining Asymmetric Solvation of Pt(II) versus Pd(II) in Aqueous Solution Revealed by Ab Initio Molecular Dynamics Simulations,
J. Chem. Theory Comput. **4**, 2108–2121 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCTC-ct800010q.pdf>`

[116] A. Witt, S. D. Ivanov, H. Forbert, and D. Marx,
Microsolvation of Protonated Methane: Structures and Energetics of $CH_5^+(H_2)_n$,
J. Phys. Chem. A **112**, 12510–12517 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JPCA-112-12510-2008.pdf>`

[115] N. N. Nair, E. Schreiner, and D. Marx,
Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions on Amino Acid Activation,
J. Am. Chem. Soc. **130**, 14148–14160 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja802370c.pdf>`

[114] N. N. Nair, E. Schreiner, R. Pollet, V. Staemmler, and D. Marx,
Magnetostructural Dynamics with the Extended Broken Symmetry Formalism: Antiferromagnetic [2Fe–2S] Complexes,
J. Chem. Theory Comput. **4**, 1174–1188 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-4-1174-2008.pdf>`

[113] M. Böckmann, N. L. Doltsinis, and D. Marx,
Azobenzene photoswitches in bulk materials,
Phys. Rev. E **78**, 036101–1-4 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRE-78-036101-2008.pdf>`

[112] M. Konôpka, R. Turanský, J. Reichert, H. Fuchs, D. Marx, and I. Štich,
Mechanochemistry and Thermochemistry are Different: Stress–Induced Strengthening of Chemical Bonds,
Phys. Rev. Lett. **100**, 115503–1-4 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-100-115503.pdf>`

[111] E. Schreiner, N. N. Nair, and D. Marx,
Influence of Extreme Thermodynamic Conditions and Pyrite Surfaces on Peptide Synthesis in Aqueous Media,
J. Am. Chem. Soc. (Communication) **130**, 2768–2770 (2008);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja7108085.pdf>`
with 17 pages of Supporting Information;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja7108085-SI.pdf>`
see also coverage in the media:
Supercomputer rekonstruiert erste Lebensmoleküle, Die Welt, Seite 31, 15.02.2008;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/peptide-welt-150208.pdf>`
Reaktionen in virtuellem Wasser, Neue Zürcher Zeitung (NZZ), 26.03.2008; NZZ–Online,

31.03.2008;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/peptide-nzz-260308.pdf>`
Bausteine des Lebens, Westdeutsche Allgemeine Zeitung (WAZ), 17.01.2009;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/peptide-waz-170109.pdf>`
Supercomputer entdeckt Bausteine des Lebens, General–Anzeiger, Seite 13, 19.02.2008;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/peptide-ga-190208.pdf>`
Präbiotische Peptidsynthese erstmals vollständig "in silico", Chemie.DE Information Service GmbH: www.bionity.com/news/d/77808/ (13.02.2008); D. Neukirchen: *Präbiotische Peptidsynthese: Chemiker untersuchen Peptidbindungen im virtuellen Labor*, Vogel Medien Gruppe (21.02.2008); *Peptidbindungen im virtuellen Labor*, Chemie Plus **3**, 8 (2008); *Chemiker untersuchen Peptidbindungen im virtuellen Labor*, LaborPraxis **3**, 14 (2008); *Präbiotische Peptidsynthese erstmals vollständig "in silico"*, BIOforum **3**, 13 (2008).

[110] E. C. Beret, R. R. Pappalardo, N. L. Doltsinis, D. Marx, and E. Sánchez Marcos,
Aqueous Pd^{II} and Pt^{II}: Anionic Hydration Revealed by Car–Parrinello Simulations,
ChemPhysChem (Communication) **9**, 237–240 (2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cpc-9-237-2008.pdf>`

[109] E. Schreiner, N. N. Nair, R. Pollet, V. Staemmler, and D. Marx,
Dynamical magnetostructural properties of Anabaena *ferredoxin,*
Proc. Natl. Acad. Sci. USA **104**, 20725–20730 (2007);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pnas2007-104-20725.pdf>` see also coverage in the media:
Magnetische Effekte in Eisen–Schwefel Proteinen, Chemie.DE Information Service GmbH: http://www.chemie.de/news/d/76026/ (21.12.2007); *Magnetische Effekte in Eisen–Schwefel–Proteinen*, Chemie Plus **1–2**, 22 (2008); *Magnetische Effekte in Eisen–Schwefel–Proteinen*, GIT Labor–Fachzeitschrift **52(2)**, 65 (2008).

[108] M. Masia, H. Forbert, and D. Marx,
Connecting Structure to Infrared Spectra of Molecular and Autodissociated HCl–Water Aggregates,
J. Phys. Chem. A **111**, 12181–12191 (2007);
part of the "Giacinto Scoles Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jp0740494.pdf>`

[107] M. Böckmann, C. Peter, L. Delle Site, N. L. Doltsinis, K. Kremer, and D. Marx,
Atomistic Force Field for Azobenzene Compounds Adapted for QM/MM Simulations with Applications to Liquids and Liquid Crystals,
J. Chem. Theory Comput. **3**, 1789–1802 (2007).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jctc-3-1789-2007.pdf>`

[106] A. Chandra, M. E. Tuckerman, and D. Marx,
Connecting Solvation Shell Structure to Proton Transport Kinetics in Hydrogen–Bonded Networks via Population Correlation Functions,
Phys. Rev. Lett. **99**, 145901-1–4 (2007).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-99-145901.pdf>`

[105] R. Kováčik, B. Meyer, and D. Marx,
F *Centers versus Dimer Vacancies on ZnO Surfaces: Characterization by STM and STS Calculations,*
Angew. Chem. Int. Ed. **46**, 4894–4897 (2007);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew46-07-4894.pdf>`
F–Zentren versus Dimerleerstellen auf ZnO–Oberflächen: Charakterisierung durch STM– und STS–Rechnungen,
Angew. Chem. **119**, 4980–4984 (2007).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew119-07-4980.pdf>`

[104] A. Chandra and D. Marx,
Creating Interfaces by Stretching the Solvent Is Key to Metallic Ammonia Solutions,
Angew. Chem. Int. Ed. **46**, 3676–3679 (2007);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew-2007-46-3676.pdf>`
Creating Interfaces by Stretching the Solvent Is Key to Metallic Ammonia Solutions,
Angew. Chem. **119**, 3750–3753 (2007).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew-2007-119-3750.pdf>`

[103] R. Pollet and D. Marx,
Ab initio *simulation of a gadolinium–based magnetic imaging contrast agent in aqueous solution,*
J. Chem. Phys. (Communication) **126**, 181102-1–3 (2007).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-Gado07.pdf>`

[102] G. Mathias and D. Marx,
Structures and spectral signatures of protonated water networks in bacteriorhodopsin,
Proc. Natl. Acad. Sci. USA **104**, 6980–6985 (2007);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PNAS-0609229104v1.pdf>`
see also coverage in the media:
V. Helms: *WLAN für die Zelle*, Physik Journal **6(6)**, 22–23 (2007);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pj-6-2007-helms.pdf>`
Wie Protonen durch die Zellmembran wandern, Chemie.DE Information Service GmbH: www.bionity.com/news/d/63769/ (19.04.2007); *Protonenwanderung: Wasser spielt eine funktionelle Rolle*, GIT Labor–Fachzeitschrift **51(6)**, 455 (2007).

[101] N. N. Nair, E. Schreiner, and D. Marx,
Glycine at the Pyrite–Water Interface: The Role of Surface Defects,
J. Am. Chem. Soc. **128**, 13815–13826 (2006);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja063295a.pdf>`
with 16 pages of Supplementary Information.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ja063295a-SI.pdf>`

[100] R. Pollet, C. Boehme, and D. Marx,
Ab Initio Simulations of Desorption and Reactivity of Glycine at a Water–Pyrite Interface at "Iron–Sulfur World" Prebiotic Conditions,
Origins Life Evol. Biospheres **36**, 363–379 (2006).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pollet-oleb2006.pdf>`

[99] B. Meyer, H. Raaba, and D. Marx,
Water adsorption on ZnO$(10\bar{1}0)$*: from single molecules to partially dissociated monolayers,*
Phys. Chem. Chem. Phys. **8**, 1513–1520 (2006);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp8-06-1513.pdf>`
see also *Cover Picture* and *Cover Story* of Themed Issue PCCP **8**(13), *1467* (2006).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-cover-full.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-cover-full.jpg>`

[98] M. E. Tuckerman, A. Chandra, and D. Marx,
Structure and Dynamics of OH^- *(aq),*
Acc. Chem. Res. **39**, 151–158 (2006);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ar040207n.pdf>`
Featured "on the ACS Publications website as a 2006 Most–Cited Article based on citation data obtained from Thomson ISI. 2006 Most–Cited Articles are articles published in 2006 receiving the most citations in the same year. ACS Publications recognizes these articles as research of immediate interest."

[97] M. Baer, E. Schreiner, A. Kohlmeyer, R. Rousseau, and D. Marx,
Inverse Temperature Transition of a Biomimetic Elastin Model: Reactive Flux Analysis of Folding/Unfolding and its Coupling to Solvent Dielectric Relaxation,
J. Phys. Chem. B **110**, 3576–3587 (2006);
part of the "Michael L. Klein Festschrift".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jp054805a.pdf>`

[96] P. Kumar P. and D. Marx,
Understanding hydrogen scrambling and infrared spectrum of bare CH_5^+ *based on* ab initio *simulations,*
Phys. Chem. Chem. Phys. **8**, 573–586 (2006).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-b513089c.pdf.pdf>`

[95] M. Benoit and D. Marx,
The Shapes of Protons in Hydrogen Bonds Depend on the Bond Length,
ChemPhysChem (Communication) **6**, 1738–1741 (2005);
part of the "Parrinello Festschrift" edited by W. Andreoni, D. Marx, and M. Sprik.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/proton-shapes-cpc.pdf>`

[94] H. Langer, N. L. Doltsinis, and D. Marx,
Excited–State Dynamics and Coupled Proton–Electron Transfer of Guanine: From the Gas Phase via Microsolvation to Aqueous Solution,
ChemPhysChem (Communication) **6**, 1734–1737 (2005);
part of the "Parrinello Festschrift" edited by W. Andreoni, D. Marx, and M. Sprik.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/gua-water-cpc.pdf>`

[93] M. Konôpka, R. Rousseau, I. Štich, and D. Marx,
Electronic Origin of Disorder and Diffusion at a Molecule–Metal Interface: Self–Assembled Monolayers Of CH_3S on Cu(111),
Phys. Rev. Lett. **95**, 096102-1–4 (2005).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL-95-096102.pdf>`

[92] O. Asvany, P. Kumar P, B. Redlich, I. Hegemann, S. Schlemmer, and D. Marx,
Understanding the Infrared Spectrum of Bare CH_5^+,
Science **309**, 1219–1222 (2005);
published online 30 June 2005 [DOI:10.1126/science.1113729] in Science*xpress* ("providing rapid electronic publication of selected Science papers based on timeliness and importance of the research");
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ch5p-lir.pdf>`
see also coverage in the media:
S. Borman: *Chemistry Highlights 2005*, Chem. & Eng. News **83(51)**, 15–20, December 19 (2005); S. Borman: *Protonated Methane Probed: Researchers obtain the first broad–frequency infrared spectrum of the CH_5^+ carbocation*, Chem. & Eng. News **83(30)**, 45–48, July 25 (2005);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ch5p-cen2005.pdf>`
G. Niedner–Schatteburg: *Im Brennpunkt: Ständig in Bewegung*, Physik Journal **4(10)**, 18–19 (2005).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ch5p-pj2005.pdf>`

[91] J. M. Stubbs and D. Marx
Aspects of Glycosidic Bond Formation in Aqueous Solution: Chemical Bonding and the Role of Water,
Chem. Eur. J. **11**, 2651–2659 (2005).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/glucose-cej.pdf>`

[90] P. R. L. Markwick, N. L. Doltsinis, and D. Marx
Targeted Car–Parrinello molecular dynamics: Elucidating double proton transfer in formic acid dimer,
J. Chem. Phys. **122**, 054112-1–8 (2005).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp-tmd-fad.pdf>`

[89] B. Meyer, D. Marx, O. Dulub, U. Diebold, M. Kunat, D. Langenberg, and Ch. Wöll
Partial Dissociation of Water Leads to Stable Superstructures on the Surface of Zinc Oxide,
Angew. Chem. Int. Ed. **43**, 6641–6645 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew43-04-6641.pdf>`
Partielle Dissoziation von Wasser führt zu stabilen Überstrukturen auf der Oberfläche von Zinkoxid,
Angew. Chem. **116**, 6809–6814 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew116-04-6809.pdf>`
see also *Cover Picture* on p. 6641.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/angew43cov-04-6641.pdf>`

[88] M. Konôpka, R. Rousseau, I. Štich, and D. Marx,
Detaching Thiolates from Copper and Gold Clusters: Which Bonds to Break ?
J. Am. Chem. Soc. **126**, 12103–12111 (2004).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cu-clus-jacs.pdf>`

[87] R. Ramírez, T. López–Ciudad, P. Kumar P, and D. Marx,
Quantum corrections to classical time–correlation functions: Hydrogen bonding and anharmonic floppy modes,
J. Chem. Phys. **121**, 3973–3983 (2004).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ir-qcf-jcp.pdf>`

[86] R. Rousseau, V. Kleinschmidt, U. W. Schmitt, and D. Marx,
Assigning Protonation Patterns in Water Networks in Bacteriorhodopsin Based on Computed IR Spectra,
Angew. Chem. Int. Ed. **43**, 4804–4807 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/br-angew-en.pdf>`
Zuordnung der Protonierungsmuster von Wassernetzwerken in Bakteriorhodopsin mittels berechneter Infrarotspektren,
Angew. Chem. **116**, 4908–4911 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/br-angew.pdf>`
see also *Cover Picture* of Bunsenmagazin (März 2004).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/br-bunsen-cover.pdf>`

[85] B. Meyer and D. Marx,
Density–functional study of Cu atoms, monolayers, films, and coadsorbates on

polar ZnO surfaces,
Phys. Rev. B **69**, 235420-1–7 (2004).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prb69-04-235420.pdf>

[84] F. Della Sala, R. Rousseau, A. Görling, and D. Marx,
Quantum and Thermal Fluctuation Effects on Photoabsorption Spectra of Clusters,
Phys. Rev. Lett. **92**, 183401-1–4 (2004).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL83401.pdf>

[83] E. Schreiner, C. Nicolini, B. Ludolph, R. Ravindra, N. Otte, A. Kohlmeyer, R. Rousseau, R. Winter, and D. Marx,
Folding and Unfolding of an Elastinlike Oligopeptide: "Inverse Temperature Transition," Reentrance, and Hydrogen–Bond Dynamics,
Phys. Rev. Lett. **92**, 148101-1–4 (2004);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prl148101.pdf>
see also *Cover Picture* and *Cover Story* of Themed Issue PCCP **6**(8), *i* (2004).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-elast-covertext.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-elast-cover.pdf>

[82] R. Rousseau, V. Kleinschmidt, U. W. Schmitt, and D. Marx,
Modeling protonated water networks in bacteriorhodopsin,
Phys. Chem. Chem. Phys. **6**, 1848–1859 (2004);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-br.pdf>
see also *Cover Picture* and *Cover Story* of Themed Issue PCCP **6**(8), *i* (2004).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-elast-covertext.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-elast-cover.pdf>

[81] R. Rousseau, E. Schreiner, A. Kohlmeyer, and D. Marx,
Temperature–Dependent Conformational Transitions and Hydrogen–Bond Dynamics of the Elastin–Like Octapeptide GVG(VPGVG): a Molecular–Dynamics Study,
Biophys. J. **86**, 1393–1407 (2004);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/Biophys_J_86_1393.pdf>
see also joint experimental paper (published "back–to–back"):
C. Nicolini, R. Ravindra, B. Ludolph, and R. Winter, *Characterization of the Temperature– and Pressure–Induced Inverse and Reentrant Transition of the Minimum Elastin–like Polypeptide GVG(VPGVG) by DSC, PPC, CD, and FT–IR Spectroscopy,* Biophys. J. **86**, 1385–1392 (2004).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/Biophys_J_86_1385.pdf>

[80] C. Boehme and D. Marx,
Glycine on a Wet Pyrite Surface at Extreme Conditions,
J. Am. Chem. Soc. (Communication to the Editor) **125**, 13362–13363 (2003).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ja0359714.pdf>

[79] J. M. Stubbs and D. Marx,
Glycosidic Bond Formation in Aqueous Solution: On the Oxocarbenium Intermediate,
J. Am. Chem. Soc. **125**, 10960–10962 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/glucose_jacs.pdf>`

[78] A. D. Boese, A. Chandra, J. M. L. Martin, and D. Marx,
From ab initio *quantum chemistry to molecular dynamics: The delicate case of hydrogen bonding in ammonia,*
J. Chem. Phys. **119**, 5965–5980 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP05965.pdf>`

[77] D. Krüger, R. Rousseau, H. Fuchs, and D. Marx,
Towards "Mechanochemistry": Mechanically Induced Isomerizations of Thiolate–Gold Clusters,
Angew. Chem. Int. Ed. **42**, 2251–2253 (2003);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew-en.pdf>`
Auf dem Weg zur "Mechano–Chemie": mechanisch induzierte Isomerisierungen von Thiolat–Goldclustern,
Angew. Chem. **115**, 2353–2355 (2003);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew.pdf>`
Featured as a *"Hot Paper"* (... "chosen by the Editors for their importance in a rapidly evolving field of high current interest");
see also *Cover Picture* on p. 2203 and *Cover Story* on p. 2205;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew-pic.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew-en-cover.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mechano-angew-cover.pdf>`
see also coverage in the media:
Virtuelles Drahtziehen: Simulierte Herstellung von Drähten mit dem Rasterkraftmikroskop, Neue Zürcher Zeitung (NZZ), 13.08.2003; Chemie Plus **7-8**, 8 (2003); Draht **5**, 13 (2003).

[76] V. Staemmler, K. Fink, B. Meyer, D. Marx, M. Kunat, S. G. Girol, U. Burghaus, and Ch. Wöll,
Stabilization of Polar ZnO Surfaces: Validating Microscopic Models by Using CO as a Probe Molecule,
Phys. Rev. Lett. **90**, 106102-1–4 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL06102.pdf>`

[75] L. Knoll, Z. Vager, and D. Marx,
Experimental versus simulated Coulomb–explosion images of flexible molecules: Structure of protonated acetylene $C_2H_3^+$*,*

Phys. Rev. A **67**, 022506-1–7 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRA22506.pdf>`

[74] H. Forbert and D. Marx,
Calculation of the permanent of a sparse positive matrix,
Comput. Phys. Commun. **150**, 267–273 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/perm_cpc.pdf>`

[73] B. Meyer and D. Marx,
First–principles study of CO adsorption on ZnO surfaces,
J. Phys.: Condens. Matter **15**, L89–L94 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcm15-03-L89.pdf>`

[72] B. Meyer and D. Marx,
Density–functional study of the structure and stability of ZnO surfaces,
Phys. Rev. B **67**, 035403-1–11 (2003).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prb67-03-035403.pdf>`

[71] B. Kirchner, J. Stubbs, and D. Marx,
Fast Anomalous Diffusion of Small Hydrophobic Species in Water,
Phys. Rev. Lett. **89**, 215901-1–4 (2002).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL15901.pdf>`

[70] D. Krüger, H. Fuchs, R. Rousseau, D. Marx, and M. Parrinello,
Pulling Monoatomic Gold Wires with Single Molecules: An Ab Initio *Simulation,*
Phys. Rev. Lett. **89**, 186402-1–4 (2002);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL86402.pdf>`
see animation `www.theochem.rub.de/go/afm.html`.

[69] M. Benoit, A. H. Romero, and D. Marx,
Reassigning Hydrogen–Bond Centering in Dense Ice,
Phys. Rev. Lett. **89**, 145501-1–4 (2002);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL45501.pdf>`
see also coverage in the media:
A. Vogel: *Geheimnis des Hochdruck–Eises entschlüsselt: Eis unter Druck*, Deutschlandfunk "Forschung Aktuell" (report and interview with D. Marx), broadcast on 24.10.2002; P. Wich: *Die Jagd nach Eis X*, Nachr. Chem. **51**, 42 (2003).

[68] M. E. Tuckerman, D. Marx, and M. Parrinello,
The nature and transport mechanism of hydrated hydroxide ions in aqueous solution,
Nature (London) **417**, 925–929 (2002);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/nature417-02-0925.pdf>`
see also the corresponding *This Week's Highlights:*

Hydroxide ions: Picture this, Nature (London) **417**, IX (2002);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/nature417-02-0925b.pdf>
see also coverage in the media:
R. Ludwig: *New Insight into the Transport Mechanism of Hydrated Hydroxide Ions in Water* ("Highlights" article), Angew. Chem. Int. Ed. **42**, 258–260 (2003); *Das Transportverhalten hydratisierter Hydroxid–Ionen in Wasser*, Angew. Chem. **115**, 268–271 (2003);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ludwig_waterm_en.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ludwig_waterm_de.pdf>
Wanderung von OH^- Defekten in Wasser: Das Rätsel basischer Lösungen, Chemie in Labor und Biotechnik, **7**, 243 (2002);
J. Schilling: *Säure–Base–Konzept: Das Ende des Tunneleffekts – Die Chemiebücher müssen umgeschrieben werden*, Chem. Rundschau **16**, 14 (2002).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/schilling_rundschau.jpg>

[67] N. L. Doltsinis and D. Marx,
Nonadiabatic Car–Parrinello molecular dynamics,
Phys. Rev. Lett. **88**, 166402-1–4 (2002);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL66402.pdf>
see animation www.theochem.rub.de/go/surfhop.html.

[66] G. M. Koretsky, M. B. Knickelbein, R. Rousseau, and D. Marx,
A Combined Infrared Photodissociation and Theoretical Study of the Interaction of Ethanol with Small Gold Clusters,
J. Phys. Chem. A **105**, 11197–11203 (2001).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jp0129636.pdf>

[65] D. Krüger, H. Fuchs, R. Rousseau, D. Marx, and M. Parrinello,
Interaction of short–chain alkane thiols and thiolates with small gold clusters: Adsorption structures and energetics,
J. Chem. Phys. **115**, 4776–4786 (2001).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP04776.pdf>

[64] M. E. Tuckerman and D. Marx,
Heavy–Atom Skeleton Quantization and Proton Tunneling in "Intermediate–Barrier" Hydrogen Bonds,
Phys. Rev. Lett. **86**, 4946–4949 (2001);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRL04946.pdf>
see animation www.theochem.rub.de/go/malon.html;
see also coverage in the media:
Animation presented at "Medienfestival – Bilder aus der Physik", IWF – Wissen und Medien Göttingen, 09.–11.11.2001; *Computer läßt Protonen tanzen*, in Ruhr–Nachrichten Bochum, 14./15.06.2001; *Protonen beim Tanzen zugeschaut*, in Verein

Deutscher Ingenieure: Ingenieur Forum Westfalen–Ruhr, p. 29, **2**/2001;*Physik: Protonentransfer im Molekül erstmals vollständig simuliert*, in dpa–Wissenschaftsdienst, p. 14–15, **25**/18.06.2001.

[63] M. Mohr, D. Marx, M. Parrinello, and H. Zipse,
Solvation of Radical Cations in Water – Reactive or Unreactive Solvation ?,
Chem. Eur. J. **6** 4009–4015 (2000).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cej_radcat.pdf>`

[62] R. Rousseau and D. Marx,
Exploring the Electronic Structure of Elemental Lithium: From Small Molecules to Nanoclusters, Bulk Metal, and Surfaces,
Chem. Eur. J. **6**, 2982–2993 (2000);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cej_lithium.pdf>`
see also *Cover Picture* on p. 2899 and *Cover Story* on p. 2901;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cej_lithium_covertext.pdf>`
see web feature `www.theochem.rub.de/go/lithium.html`.

[61] L. Knoll and D. Marx,
Molecular structure calculations via path integral simulations: Estimating finite–discretization errors,
Eur. Phys. J. D **10**, 353–362 (2000).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/epjd00100353.pdf>`

[60] D. Marx, M. E. Tuckerman, and M. Parrinello,
Solvated excess protons in water: quantum effects on the hydration structure,
J. Phys.: Condens. Matter **12**, A153–A159 (2000).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcmc00h17.pdf>`

[59] R. Rousseau and D. Marx,
The interaction of gold clusters with methanol molecules: Ab initio *molecular dynamics of* $Au_n^+CH_3OH$ *and* Au_nCH_3OH,
J. Chem. Phys. **112**, 761–769 (2000);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP00761.pdf>`
see also joint experimental paper (published "back–to–back"):
G. Dietrich, S. Krückeberg, K. Lützenkirchen, L. Schweikhard, and C. Walther,
The interaction of gold clusters with methanol molecules: Infrared photodissociation of mass–selected $Au_n^+(CH_3OH)_m$, J. Chem. Phys. **112**, 752–760 (2000).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP00752.pdf>`

[58] D. Marx and M. Parrinello,
CH_5^+ *Stability and Mass Spectrometry*,
Science **286**, 1051 (1999); DOI:10.1126/science.286.5442.1051a;

Anonymous ftp: <outgoing/dominik_marx/PAPERS/science1051a.pdf>
see also www.sciencemag.org/cgi/content/full/286/5442/1051a.

[57] R. Rousseau and D. Marx,
The role of quantum and thermal fluctuations upon properties of lithium clusters,
J. Chem. Phys. **111**, 5091–5101 (1999).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/JCP05091.pdf>

[56] I. Frank, D. Marx, and M. Parrinello,
First–Principles Molecular Dynamics Study of a Photochromic Molecular Crystal,
J. Phys. Chem. A **103**, 7341–7344 (1999).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jpca991238g.pdf>

[55] M. Benoit, D. Marx, and M. Parrinello,
The role of quantum effects and ionic defects in high–density ice,
Solid State Ionics **125**, 23–29 (1999).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ssi125-99-0023.pdf>

[54] D. Marx, M. E. Tuckerman, and G. J. Martyna,
Quantum dynamics via adiabatic ab initio centroid molecular dynamics,
Comput. Phys. Commun. **118**, 166–184 (1999).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpc118-99-0166.pdf>

[53] D. Marx, M. E. Tuckerman, J. Hutter, and M. Parrinello,
The nature of the hydrated excess proton in water,
Nature (London) **397**, 601–604 (1999);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/nature397-99-601.pdf>
see also corresponding *News & Views* article: J. T. Hynes: *The protean proton in water* in Nature (London) **397**, 565–567 (1999);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/nature397-99-565.pdf>
see also coverage in the media:
Spektrum der Wissenschaft: Ticker "Meldung des Tages" on 19.02.1999; D. Busath: *Short Review* in Molecular Modeling & Computational Chemistry **8**, 2 (1999); S. Albus: *Protonenrennen im Säurebett* in Süddeutsche Zeitung, 16.03.1999, S. V2/12; M. Rauner: *Schnelle Protonen* in Phys. Bl. **55**, 17–18 (1999).

[52] R. Rousseau, G. Dietrich, S. Krückeberg, K. Lützenkirchen, D. Marx, L. Schweikhard, and C. Walther,
Probing cluster structures with sensor molecules: methanol adsorbed onto gold clusters,
Chem. Phys. Lett. **295**, 41–46 (1998).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpl295-98-0041.pdf>

[51] S. Biermann, D. Hohl, and D. Marx,
Quantum Effects in Solid Hydrogen at Ultra–High Pressure,
Solid State Commun. **108**, 337–341 (1998).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ssc108-98-0337.pdf>`

[50] M. Benoit, D. Marx, and M. Parrinello,
Tunnelling and zero–point motion in high–pressure ice,
Nature (London) **392**, 258–261 (1998);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/nature392-98-258.pdf>`
see also corresponding *News & Views* article: J. Teixeira: *The double identity of ice X*; Nature (London) **392**, 232–233 (1998);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/nature392-98-232.pdf>`
see also coverage in the media:
Süddeutsche Zeitung, 09.04.1998, S. 22; La Recherche **309** p. 16, May 1998.

[49] R. Rousseau and D. Marx,
Fluctuations and Bonding in Lithium Clusters,
Phys. Rev. Lett. **80**, 2574–2577 (1998);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/PRL02574.pdf>`
see web feature `www.theochem.rub.de/go/lithium.html`.

[48] I. Frank, J. Hutter, D. Marx, and M. Parrinello,
Molecular dynamics in low–spin excited states,
J. Chem. Phys. **108**, 4060–4069 (1998).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp_roks.pdf>`

[47] S. Biermann, D. Hohl, and D. Marx,
Proton Quantum Effects in High Pressure Hydrogen,
J. Low Temp. Phys. **110**, 97–102 (1998).

[46] M. Benoit, D. Marx, and M. Parrinello,
Quantum effects on phase transitions in high–pressure ice,
Comp. Mat. Sci. **10**, 88–93 (1998).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cms10-98-0088.pdf>`

[45] M. Mohr, H. Zipse, D. Marx, and M. Parrinello,
Interaction of Alkene Radical Cations with Solvent Molecules as Described with Density Functional Theory,
J. Phys. Chem. A **101**, 8942–8948 (1997).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca972344q.pdf>`

[44] I. Štich, D. Marx, M. Parrinello, and K. Terakura,
Protonated hydrogen clusters,

J. Chem. Phys. **107**, 9482–9492 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/jcp_phydrogenclust.pdf>

[43] D. Marx and A. Savin,
Topological Bifurcation Analysis: Electronic Structure of CH_5^+,
Angew. Chem. Int. Ed. Engl. **36**, 2077–2080 (1997);
Topologische Bifurkationsanalyse: Elektronenstruktur von CH_5^+,
Angew. Chem. **109**, 2168–2170 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ch5p_angewandte.pdf>

[42] D. Marx and M. Parrinello,
Structure and dynamics of protonated methane: CH_5^+ *at finite temperatures*,
Z. Phys. D **41**, 253–260 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/zpd70410253.pdf>

[41] D. Marx, M. Sprik, and M. Parrinello,
Ab initio molecular dynamics of ion solvation. The case of Be^{2+} *in water*,
Chem. Phys. Lett. **273**, 360–366 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpl273-97-0360.pdf>

[40] R. Rousseau and D. Marx,
Ab initio calculations on small lithium clusters,
Phys. Rev. A **56**, 617–625 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/PRA617_1.pdf>

[39] A. C. Mitus, H. Weber, and D. Marx,
Local structure analysis of the hard–disk fluid near melting,
Phys. Rev. E **55**, 6855–6859 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pre55-97-6855.pdf>

[38] I. Štich, D. Marx, M. Parrinello, and K. Terakura,
Proton–Induced Plasticity of Hydrogen Clusters,
Phys. Rev. Lett. **78**, 3669–3672 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/prl3669_1.pdf>

[37] R. Martoňák, D. Marx, and P. Nielaba,
Quantum fluctuations driven orientational disordering: A finite–size scaling study,
Phys. Rev. E **55**, 2184–2194 (1997).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pre55-97-2184.pdf>

[36] M. E. Tuckerman, D. Marx, M. L. Klein, and M. Parrinello,
On the Quantum Nature of the Shared Proton in Hydrogen Bonds,
Science **275**, 817–820 (1997);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/science275-97-0817.pdf>
see also the corresponding highlight in Science **275**, 729 (1997).

[35] H. Weber and D. Marx,
Comment on "One–Stage Continuous Melting Transition in Two Dimensions",
Phys. Rev. Lett. **78**, 398 (1997).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prl78-97-398.pdf>`

[34] M. E. Tuckerman, D. Marx, M. L. Klein, and M. Parrinello,
Efficient and general algorithms for path integral Car–Parrinello molecular dynamics,
J. Chem. Phys. **104**, 5579–5588 (1996).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp104-96-5579.pdf>`

[33] D. Marx and M. Parrinello,
Ab initio *path integral molecular dynamics: Basic ideas*,
J. Chem. Phys. **104**, 4077–4082 (1996).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp104-96-4077.pdf>`

[32] I. Frank, D. Marx, and M. Parrinello,
Structure and electronic properties of quinizarin chemisorbed on alumina,
J. Chem. Phys. **104**, 8143–8150 (1996).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jcp104-96-8143.pdf>`

[31] D. Marx and M. Parrinello,
The Effect of Quantum and Thermal Fluctuations on the Structure of the Floppy Molecule $C_2H_3^+$,
Science **271**, 179–181 (1996).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/science271-96-0179.pdf>`

[30] D. Marx, E. S. Fois, and M. Parrinello,
Static and Dynamic Density Functional Investigation of Hydrated Beryllium Dications,
Int. J. Quantum Chem. **57**, 655–662 (1996).

[29] E. Ermakova, J. Solca, H. Huber, and D. Marx,
Many–body and quantum effects in the radial distribution function of liquid neon and argon,
Chem. Phys. Lett. **246**, 204–208 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cpl246-95-0204.pdf>`

[28] I. Frank, D. Marx, and M. Parrinello,
First Principles Investigation of Quinizarin Chemisorbed on α*–*Al_2O_3,
J. Am. Chem. Soc. (Communication to the Editor) **117**, 8037–8038 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jacs117-95-8037.pdf>`

[27] D. Marx, J. Hutter, and M. Parrinello,
Density functional study of small aqueous Be^{2+} *clusters*,

Chem. Phys. Lett. **241**, 457–462 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cpl241-95-0457.pdf>`

[26] D. Marx and M. Parrinello,
Structural quantum effects and three–centre two–electron bonding in CH_5^+,
Nature (London) **375**, 216–218 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/nature375-95-216.pdf>`

[25] H. Weber, D. Marx, and K. Binder,
On the melting transition in two dimensions: a finite–size scaling analysis of bond–orientational order in hard discs,
Phys. Rev. B **51**, 14636–14651 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prb51-95-14636.pdf>`

[24] D. Marx and P. Nielaba,
Quantum "melting" of orientationally ordered physisobates,
J. Chem. Phys. **102**, 4538–4547 (1995).

[23] F. Schneider, D. Marx, and P. Nielaba,
Gibbs–ensemble path–integral Monte Carlo simulations of a mixed quantum–classical fluid,
Phys. Rev. E **51**, 5162–5165 (1995).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pre51-95-5162.pdf>`

[22] H. Weber and D. Marx,
Two–Dimensinal Melting Approached via Finite–Size Scaling of Bond–Orientational Order,
Europhys. Lett. **27**, 593–598 (1994).

[21] D. Marx, S. Sengupta, P. Nielaba, and K. Binder,
Monte Carlo investigation of head–tail ordering of CO monolayers on graphite,
Surf. Sci. **321**, 195–216 (1994).

[20] D. Marx, S. Sengupta, O. Opitz, P. Nielaba, and K. Binder,
N_2 monolayers physisorbed on graphite: The herringbone transition revisited,
Mol. Phys. **83**, 31–62 (1994).

[19] D. Marx and M. Parrinello,
Ab initio path–integral molecular dynamics,
Z. Phys. B (Rapid Note) **95**, 143–144 (1994).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/zpb95-94-143.pdf>`

[18] D. Marx,
Rotational motion of linear molecules in three dimensions: A path-integral Monte

Carlo approach,
Mol. Simulat. **12**, 33–48 (1994).

[17] S. Sengupta, D. Marx, P. Nielaba, and K. Binder,
Phase diagram of a model anticlustering binary mixture in two dimensions: A semi–grand–canonical Monte Carlo study,
Phys. Rev. E **49**, 1468–1477 (1994).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pre49-94-1468.pdf>`

[16] D. Marx, S. Sengupta, and P. Nielaba,
Quantum Effects and Orientational Ordering in Adsorbed Layers of Linear Molecules,
Ber. Bunsenges. Phys. Chem. **98**, 525–527 (1994).

[15] D. Marx, S. Sengupta, P. Nielaba, and K. Binder,
The phase diagram of a two–dimensional fluid with internal quantum states,
J. Phys.: Condens. Matter **6**, A175–A180 (1994).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cm942c25.pdf>`

[14] D. Marx, S. Sengupta, P. Nielaba, and K. Binder,
Clarification of the Head–Tail Ordering of CO on Graphite: A Monte Carlo Study,
Phys. Rev. Lett. **72**, 262–265 (1994).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prl72-94-262.pdf>`

[13] A. C. Mitus, D. Marx, S. Sengupta, P. Nielaba, A. Z. Patashinskii, and H. Hahn,
Locating liquid–solid transitions in computer simulations based on local structure analysis,
J. Phys.: Condens. Matter **5**, 8509–8522 (1993).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cm934503.pdf>`

[12] S. Sengupta, O. Opitz, D. Marx, and P. Nielaba,
Herringbone Orientational Transition in Monolayer N_2 Adsorbed on Graphite by Density Functional Theory,
Europhys. Lett. **24**, 13–19 (1993).

[11] O. Opitz, D. Marx, S. Sengupta, P. Nielaba, and K. Binder,
On the order of the herringbone transition of N_2 on graphite: a Monte Carlo study,
Surf. Sci. Lett. **297**, L122–L126 (1993).

[10] D. Marx, S. Sengupta, and P. Nielaba,
Diatomic molecules, rotations, and path-integral Monte Carlo simulations: N_2 and H_2 on graphite,
J. Chem. Phys. **99**, 6031–6051 (1993).

[9] D. Marx, O. Opitz, P. Nielaba, and K. Binder,
Quantum Effects on the Herringbone Ordering of N_2 on Graphite,

Phys. Rev. Lett. **70**, 2908–2911 (1993).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prl70-93-2908.pdf>`

[8] D. Marx, P. Nielaba, and K. Binder,
Path-integral Monte Carlo study of a model adsorbate with internal quantum states,
Phys. Rev. B **47**, 7788–7804 (1993).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prb47-93-7788.pdf>`

[7] S. Sengupta, D. Marx, and P. Nielaba,
Density Functional Theory of Magnetization–Driven Phase Transitions in Fluids with Internal Quantum States,
Europhys. Lett. **20**, 383–388 (1992).

[6] D. Marx and P. Nielaba,
Path-integral Monte Carlo techniques for rotational motion in two dimensions: Quenched, annealed, and nospin quantum–statistical averages,
Phys. Rev. A **45**, 8968–8971 (1992).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pra45-92-8968.pdf>`

[5] D. Marx,
Phase diagram of a model adsorbate with internal quantum states,
Surf. Sci. **272**, 198–203 (1992).

[4] D. Marx, P. Nielaba, and K. Binder,
On the calculation of the heat capacity in path-integral Monte Carlo simulations,
Int. J. Mod. Phys. C **3**, 337–346 (1992).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ijmpc-3-92-337.pdf>`

[3] D. Marx, P. Nielaba, and K. Binder,
Phase transitions in Two–Dimensional Fluids with Internal Quantum States,
Phys. Rev. Lett. **67**, 3124–3127 (1991).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prl67-91-3124.pdf>`

[2] D. Marx, K. Heinzinger, G. Pálinkás, and I. Bakó,
Structure and Dynamics of NaCl in Methanol. A Molecular Dynamics Study,
Z. Naturforsch. **46a**, 887–897 (1991).

[1] D. Marx, D. Kleinhesselink, and M. Wolfsberg,
A Note on Some Reported C and N Isotope Effects,
J. Am. Chem. Soc. (Communication to the Editor) **111**, 1493–1494 (1989).

2 Invited Reviews, Features, Comments, and Lecture Notes

[R35] D. Munoz–Santiburcio and D. Marx,
Confinement-Controlled Aqueous Chemistry within Nanometric Slit Pores,
Chem. Rev. **121**, 6293–6320 (2021).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/cr-2021-121-6293.pdf>`

[R34] F. Brieuc, C. Schran, F. Uhl, H. Forbert, and D. Marx,
Converged quantum simulations of reactive solutes in superfluid helium: The Bochum perspective,
J. Chem. Phys. (Perspective Article) **152**, 210901-1–22 (2020);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2020-152-210901.pdf>`
see also *Cover Picture*;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/JCP-2020-152-210901-cov.pdf>`

[R33] D. Marx,
Comment on "Inter/Intramolecular Bonds in TH_5^+ (T = C/Si/Ge): H_2 as Tetrel Bond Acceptor and the Uniqueness of Carbon Bonds",
J. Phys. Chem. A (Comment) **123**, 9240–9241 (2019).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpca-2019-123-9240.pdf>`

[R32] K. Morgenstern, D. Marx, M. Havenith, and M. Muhler,
Solvation Science (Editorial of PCCP Themed Issue),
Phys. Chem. Chem. Phys. **17**, 8295–8296 (2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c5cp90022k.pdf>`

[R31] C. Drechsel–Grau and D. Marx,
Tunneling in chiral water clusters: Protons in concert (News and Views Article),
Nat. Phys. **11**, 216–218 (2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/naturephys-2015-11-216.pdf>`

[R30] V. Staemmler, C. Hättig, and D. Marx, (Guest Editors),
Editorial: Special Issue in Honour of Professor Kutzelnigg,
Mol. Phys. **111**, 2375–2376 (2013).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mol-phys-editorial.pdf>`

[R29] S. D. Ivanov, A. Witt, and D. Marx,
Theoretical spectroscopy using molecular dynamics: theory and application to CH_5^+ and its isotopologues (Perspective Article),
Phys. Chem. Chem. Phys. **15**, 10270–10299 (2013);
part of the PCCP Themed Issue "Theory meets Spectroscopy".
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-2013-15-10270.pdf>`

[R28] J. Frenzel, J. Kiss, N. N. Nair, B. Meyer, and D. Marx,
Methanol synthesis on ZnO from molecular dynamics (Feature Article),

Phys. Status Solidi B **250**, 1174–1190 (2013);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pssb-2013-250-1174.pdf> ee also *Backcover Picture*.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pssb-2013-250-1174-cover.pdf>

[R27] P. Dopieralski, P. Anjukandi, J. Ribas–Arino, and D. Marx,
Theoretical Mechanochemistry: Stressing Molecules in the "Virtual Lab",
inSiDE (Innovatives Supercomputing in Deutschland) **10(2)**, 48–53 (2012).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/inside-cmc-2012.pdf>

[R26] J. Ribas–Arino and D. Marx,
Covalent Mechanochemistry: Theoretical Concepts and Computational Tools with Applications to Molecular Nanomechanics,
Chem. Rev. **112**, 5412–5487 (2012);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cmc-chemrev-2012.pdf>
see also coverage in the media:
B. Halford, *Tugging on Molecules (Mechanochemistry: When molecules meet force)*, Chem. & Eng. News **90(40)**, 55–57, October 1 (2012);
http://cen.acs.org/magazine/90/09040.html
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cmc-feature-cen-2012.pdf>

[R25] A. Witt, S. D. Ivanov, and D. Marx,
Dem Geheimnis einer "Supersäure" auf der Spur (Invited Feature Article for Public Outreach),
Akademie Aktuell **41**, 66–69 (2012);
http://www.badw.de/aktuell/akademie_aktuell/2012/heft2/index.html
Anonymous ftp: <outgoing/dominik_marx/PAPERS/AA-41-66-2012.pdf>

[R24] R. Glaves, G. Mathias, and D. Marx,
"In Silico" Phosphate Transfer: From Bulk Water to Enzymes,
inSiDE (Innovatives Supercomputing in Deutschland) **10(1)**, 40–43 (2012); Erratum: **10(2)**, 112 (2012).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/inside-2012.pdf>

[R23] M. Böckmann, D. Marx, C. Peter, L. Delle Site, K. Kremer, and N. L. Doltsinis,
Multiscale modelling of mesoscopic phenomena triggered by quantum events: light–driven azo–materials and beyond (Perspective Article),
Phys. Chem. Chem. Phys. **13**, 7604–7621 (2011).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-13-2011-7604.pdf>

[R22] D. Marx, A. Chandra, and M. E. Tuckerman,
Aqueous Basic Solutions: Hydroxide Solvation, Structural Diffusion, and Comparison to the Hydrated Proton,
Chem. Rev. **110**, 2174–2216 (2010).

Anonymous ftp: <outgoing/dominik_marx/PAPERS/cr900233f.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cr900233f+cov.pdf>

[R21] M. Konôpka, R. Turanský, N. L. Doltsinis, D. Marx, and I. Štich,
Organometallic Nanojunctions Probed by Different Chemistries: Thermo–, Photo–, and Mechano–Chemistry,
Adv. Solid State Phys. **48**, 219–235 (2009).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/ASSP-48-219-2009.pdf>

[R20] N. N. Nair, E. Schreiner, and D. Marx,
Prebiotic Peptide Synthesis on Blue Gene Platforms at "Iron–Sulfur–World" Conditions,
INSIDE (Innovatives Supercomputing in Deutschland) **6(2)**, 30–35 (2008).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/inside-2008.pdf>

[R19] H. Fuchs, D. Marx, and U. Simon,
Analysis, manipulation, and simulation on the nanoscale (Editorial of PCCP Themed Issue),
Phys. Chem. Chem. Phys. **10**, 1841–1843 (2008).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-nano08.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/pccp-nano08-cov.eps>

[R18] H. Fuchs, D. Marx, and U. Simon,
Analyse, Manipulation und Simulation auf der Nanoskala (Leitartikel zur 107. Hauptversammlung der Deutschen Bunsen–Gesellschaft für Physikalische Chemie),
Bunsen–Magazin, No. 2 (März), 44–45 (2008).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/bunsen-nano08.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/bunsen-nano08-cov.eps>

[R17] D. Marx,
Advanced Car–Parrinello Techniques: Path Integrals and Nonadiabaticity in Condensed Matter Simulations,
Lect. Notes Phys. **704**, 507–539 (2006).
Anonymous ftp: <outgoing/dominik_marx/PAPERS/marx-erice06.pdf>

[R16] D. Marx,
Proton Transfer 200 Years after von Grotthuss: Insights from Ab Initio Simulations (Review Article),
ChemPhysChem **7**, 1848–1870 (2006);
Addendum: ChemPhysChem **8**, 209–210 (2007);
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpc-rev06.pdf>
Invited Review by the Editors; see also *Cover Picture* and *Cover Story* on p. 1837.
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpc-rev06-cover.pdf>
Anonymous ftp: <outgoing/dominik_marx/PAPERS/cpc-rev06-coverpic.pdf>

[R15] D. Marx,
An Introduction to Ab Initio Molecular Dynamics Simulations,
in *Computational Nanoscience: Do It Yourself!*, pp.195–244,
Editors: J. Grotendorst, S. Blügel, and D. Marx (John von Neumann Institute for Computing, Forschungszentrum Jülich 2006); for downloads see
`www.theochem.rub.de/go/cprev.html` or
`www2.fz-juelich.de/nic-series/volume31/marx.pdf`.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/wscn-2006.pdf>`

[R14] W. Andreoni, D. Marx, and M. Sprik,
A Tribute to Michele Parrinello: From Physics via Chemistry to Biology (Editorial of the "Parrinello Festschrift"),
ChemPhysChem **6**, 1671–1676 (2005);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-tribute.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-festschrift-lr.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-festschrift-hr.pdf>`
see also *Cover Picture* and *Cover Story* on p. 1685.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover-hr.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover-text.pdf>`

[R13] D. Marx,
Wasser, Eis und Protonen: Mit Quantensimulationen zum molekularen Verständnis von Wasserstoffbrücken, Protonentransfer und Phasenübergängen,
Physik Journal **3(5)**, 33–39 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pj-protonen.pdf>`
Invited Overview Article by Deutsche Physikalische Gesellschaft DPG (German Physical Society) in the Special Issue "Computational Physics";
see also *Cover Picture* and *Cover Story* on p. 4–5.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pj-cover.ps>`

[R12] D. Marx,
Theoretical Chemistry in the 21st Century: The "Virtual Lab",
in *Proceedings of the "Idea–Finding Symposium: Frankfurt Institute for Advanced Studies"*, pp. 139–153,
Editors: W. Greiner and J. Reinhardt (EP Systema, Debrecen, 2004).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/fias-marx.pdf>`

[R11] D. Marx,
Throwing Tetrahedral Dice (Perspective Article),
Science **303**, 634–636 (2004);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/marx-ws-science.ps>`

`<outgoing/dominik_marx/PAPERS/science-303-5658-634.pdf>`
Invited Perspective Article "Interfacial Water / Chemistry".

[R10a] N. L. Doltsinis, W. Sander und D. Marx,
Photochemische Reaktionen im "virtuellen Labor": Vom Lichtblitz zum Lichtblick,
ChemieRUBIN – Das Wissenschaftsmagazin der RUB (2003), S. 33–37;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemrubin-photo.pdf>`
see also coverage in the media:
U. Schulte, *Photoreaktionen im Molekül,* Deutsche Apotheker Zeitung **144**(12), 1341–1343 (18.03.2004); A. Rooch, *Chemiker lassen Moleküle tanzen,* Westdeutsche Allgemeine Zeitung, 22.05.2004.

[R10b] H. Weingärtner und D. Marx,
Wasser – mehr als ein Lösungsmittel: Das Eis ist heiß,
ChemieRUBIN – Das Wissenschaftsmagazin der RUB (2003), S. 22–27.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/chemrubin-wasser.pdf>`

[R9] N. L. Doltsinis and D. Marx,
First Principles Molecular Dynamics Involving Excited States and Nonadiabatic Transitions,
J. Theor. Comput. Chem. **1**, 319–349 (2002);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/nacp-rev_jtcc.pdf>`
Invited Topical Review for the *Inaugural Volume* of "Journal of Theoretical and Computational Chemistry" (JTCC); for downloads see
`www.theochem.rub.de/go/cprev.html`.

[R8] D. Marx and J. Hutter,
Ab Initio Molecular Dynamics: Theory and Implementation,
in *Modern Methods and Algorithms of Quantum Chemistry*, pp. 301–449 (first edition, paperback, ISBN 3–00–005618–1) or pp. 329–477 (second edition, hardcover, ISBN 3–00–005834–6),
Editor: J. Grotendorst (John von Neumann Institute for Computing, Forschungszentrum Jülich 2000); for downloads see
`www.theochem.rub.de/go/cprev.html` or
`www2.fz-juelich.de/nic-series/Volume3/marx.ps` or `/marx.pdf`.

[R7] D. Marx,
Protonenwanderung im virtuellen Labor,
Spektrum der Wissenschaft (German edition of *Scientific American*), pp. 21–25, Juli 1999;
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/grotthuss.pdf>`
Spektrum der Wissenschaft DIGEST: *Moderne Chemie II / Chemie und Computer*, pp. 68–71, 1 / 2000;

see also coverage in the media: G. Latzel, *Zur Wirkungsweise des PEM–Feststoff–Elektrolyten*, Praxis der Naturwissenschaften – Chemie in der Schule **49(8)**, 10–12 (2000).

[R6] D. Marx,
"Ab initio liquids": Simulating liquids based on first principles,
in *New Approaches to Problems in Liquid State Theory*, pp. 439–457,
Editors: C. Caccamo, J.–P. Hansen, and G. Stell (Kluwer, Dordrecht 1999).

[R5] D. Marx and M. Parrinello,
CH_5^+: The Cheshire Cat Smiles,
Science **284**, 59–60 (1999);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/ch5p_science.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/science284-99-0059.pdf>`
Invited Perspective Article "Molecular Spectroscopy";
for further discussions see: *CH_5^+ Stability and Mass Spectrometry*, Comment by G. M. Kramer, Response by T. Oka and E. T. White and D. Marx and M. Parrinello, Science **286**, 1051 (1999);
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/science1051a.pdf>`
for downloads see `www.sciencemag.org/cgi/content/full/286/5442/1051a.`

[R4] D. Marx,
Simulationen vom Car–Parrinello–Typ (Trendbericht Theoretische Chemie 1998), Nachr. Chem. Tech. Lab. **47**, 186–188 (1999).

[R3] D. Marx and M. H. Müser,
Path integral simulations of rotors: theory and applications,
J. Phys.: Condens. Matter **11**, R117–R155 (1999).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/jpcmc911r1.pdf>`

[R2] D. Marx,
Proton transfer in ice,
in *Classical and Quantum Dynamics in Condensed Phase Simulations*, Chapt. 15, pp. 359–383,
Editors: B. J. Berne, G. Ciccotti, and D. F. Coker (World Scientific, Singapore 1998).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/lerici_lecture.pdf>`

[R1] D. Marx and H. Wiechert,
Ordering and Phase Transitions in Adsorbed Monolayers of Diatomic Molecules,
Adv. Chem. Phys. **95**, 213–394 (1996).

3 Monographs

[M1] D. Marx and J. Hutter,
Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods,
(Cambridge University Press, Cambridge 2009);

ISBN: 978–0–521–89863–8, Hardback, 578 pages, 1669 references;
CUP Homepage: `http://www.cambridge.org/9780521898638`;

(Cambridge University Press, Cambridge 2012, paperback reprint);
ISBN: 978–1–107–66353-4, Paperback, 578 pages, 1669 references;
CUP Homepage: `http://www.cambridge.org/9781107663534`;
Errata and Addenda: `http://www.theochem.rub.de/go/aimd-book.html`.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/aimd-look-inside.pdf>`
Cover page:
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/aimd-cover-lowres.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/aimd-cover-highres.pdf>`

4 Edited Books and Special Issues

[B9] K. Morgenstern, D. Marx, M. Havenith, and M. Muhler, (Guest Editors),
Solvation Science (Themed Issue),
Phys. Chem. Chem. Phys. Volume **17**, Number 13, Pages 8285–8540 (April 7, 2015).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c5cp90022k.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/c5cp90045j.pdf>`

[B8] G. Sutmann, J. Grotendorst, G. Gompper, and D. Marx, (Editors),
Computational Trends in Solvation and Transport in Liquids (VI+614 pages),
(Institute for Advanced Simulation and Jülich Supercomputing Centre, Forschungszentrum Jülich 2015);
Printed Hardcover Version: `ISBN 978-3-95806-030-2`
Electronic Version:
`https://juser.fz-juelich.de/record/188877/files/IAS-Band-28-V2.pdf`
`http://www.fz-juelich.de/conferences/STL-2015/EN/Publications/_node.html`

[B7] V. Staemmler, C. Hättig, and D. Marx, (Guest Editors),
Special Issue in Honour of Professor Kutzelnigg,
Mol. Phys. Volume **111**, Issues 16–17, Pages 2375–2662 (2013).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/mol-phys-editorial.pdf>`

[B6] J. Grotendorst, G. Sutmann, G. Gompper, and D. Marx, (Editors),
Hierarchial Methods for Dynamics in Complex Molecular Systems (VI+540 pages),
(Institute for Advanced Simulation and Jülich Supercomputing Centre, Forschungszentrum Jülich 2012);
Printed Hardcover Version: `ISBN 978-3-89336-768-9`
Electronic Version:
`http://juser.fz-juelich.de/record/127337/files/IAS-Series-10.pdf`

[B5] J. Grotendorst, N. Attig, S. Blügel, and D. Marx, (Editors),
Multiscale Simulation Methods in Molecular Sciences (VI+569 pages),
(Institute for Advanced Simulation and Jülich Supercomputing Centre, Forschungszentrum Jülich 2009);
Printed Hardcover Version: `ISBN 978-3-9810843-8-2`
Electronic Version: `www2.fz-juelich.de/nic-series/volume42/`

[B4] H. Fuchs, D. Marx, and U. Simon, (Guest Editors),
Analysis, manipulation, and simulation on the nanoscale (Themed Issue),
Phys. Chem. Chem. Phys. Volume **10**, Number 14, Pages 1841–1982 (April 14, 2008).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-nano08.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/pccp-nano08-cov.eps>`

[B3] J. Grotendorst, S. Blügel, and D. Marx, (Editors),
Computational Nanoscience: Do It Yourself! (V+522 pages),
(John von Neumann Institute for Computing, Forschungszentrum Jülich 2006);
Printed Hardcover Version: `ISBN 3-00-017350-1`
Electronic Version: `www2.fz-juelich.de/nic-series/volume31/`

[B2] W. Andreoni, D. Marx, and M. Sprik, (Guest Editors),
Parrinello Festschrift: From Physics via Chemistry to Biology (Special Issue),
ChemPhysChem Volume **6**, Issue 9, Pages 1671–1947 (September 12, 2005).
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-festschrift-lr.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-festschrift-hr.pdf>`
see also *Cover Picture* and *Cover Story* on p. 1685.
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover-hr.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover.pdf>`
Anonymous ftp: `<outgoing/dominik_marx/PAPERS/prr-cover-text.pdf>`

[B1] J. Grotendorst, D. Marx, and A. Muramatsu, (Editors),
Quantum Simulations of Complex Many–Body Systems: From Theory to Algorithms (V+548 pages),
(John von Neumann Institute for Computing, Forschungszentrum Jülich 2002);
Printed Hardcover Version: `ISBN 3-00-009057-6`

Electronic Version: www2.fz-juelich.de/nic-series/volume10/
Audio–Visual Lecture Notes: www2.fz-juelich.de/video/wsqs/