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Publikationsverzeichnis – List of publications

90 [Poly \(hexamethylene biguanide\) adsorption on hydrogen peroxidetreated Ti-Al-V alloys and effects on wettability, antimicrobialefficacy, and cytotoxicity](#)

Gerald Müller , Hicham Benkhai , Rutger Matthes , Birgit Finke , Wenke Friedrichs, Norman Geist , Walter Langel , Axel Kramer, Biomaterials xxx (2014) 1-17

89 [Titanium binding dodecapeptides and the impact of water structure](#)

Wenke Friedrichs, Susan Köppen, Walter Langel, Surface Science 617 (2013) 42–52

88 [Role of nitrogen in evolution of sp²/sp³ bonding and optical band gap in hydrogenated carbon nitride](#)

Majumdar, Abhijit; Das, Sadhan Chandra; Bogdanowicz, Robert; Shripathi, Thoudinja; Langel, Walter; Hippler, Rainer
Vibrational Spectroscopy (2013), 66, 63-68

87 [DFT Simulations of Titanium Oxide Films on Titanium Metal](#)

B. Ohler, S. Prada, G. Pacchioni, W. Langel,
J Phys Chem C (2013), 117(1), 358-367

86 [Substrate-Enzyme Interaction in Pig Liver Esterase](#)

Hasenpusch, D.; Moeller, D.; Bornscheuer, U. T.; Langel, W.
arXiv.org, e-Print Archive, Quantitative Biology (2012), 1-32, arXiv:1204.6186v1 [q-bio.BM].

85 [Adsorption of Collagen Nanofibrils on Rough TiO₂: A Molecular Dynamics Study](#)

W. Friedrichs, B. Ohler, W. Langel, S. Monti, S. Köppen
Advanced Engineering Materials (2011) [13](#) B334–B3422011

84 [Molecular dynamics studies of changes in the DNA-structure as result of interactions with cisplatin](#)

Issanin, A. N.; Langel, W.; Bednarski, P. J.
arXiv.org, e-Print Archive, Quantitative Biology (2011), 1-7, arXiv:1107.3921v1

83 [Simulation on the structure of pig liver esterase](#)

Hasenpusch, D.; Bornscheuer, U. T.; Langel, W.

J Mol Mod (2011), 17, 1493-1506. DOI:10.1007/s00894-010-0846-x

82 [Simulation of Adhesion Forces and Energies of Peptides on Titanium Dioxide Surfaces](#)

Koeppen, S.; Langel, W.

Langmuir (2010), 26, 15248-15256. DOI:10.1021/la101687m

81 [NMR structural studies on the covalent DNA binding of a pyrrolobenzodiazepine-naphthalimide conjugate](#)

Rettig, M.; Langel, W.; Kamal, A.; Weisz, K.

Organic & Biomolecular Chemistry (2010), 8, 3179-3187. DOI:10.1039/c001893g

80 [Measurement of adsorption isotherms in the gas phase on native titanium dioxide surfaces by quartz crystal microbalance technique](#)

Marx, A.; Langel, W.

J Vac Sci Tech, A: (2010), 28, 232-237. DOI:10.1116/1.3294716

79 [Solution Structure of a Covalently Bound Pyrrolo\[2,1-c\]\[1,4\]benzodiazepine-Benzimidazole Hybrid to a 10mer DNA Duplex](#)

Rettig, M.; Weingarth, M.; Langel, W.; Kamal, A.; Kumar, P. P.; Weisz, K.

Biochemistry (2009), 48, 12223-12232. DOI:10.1021/bi901655t

78 [Molecular dynamics simulations on the interface between titanium dioxide and water droplets. A new model for the contact angle](#)

Ohler, B.; Langel, W.

J Phys Chem C (2009), 113, 10189-10197. DOI:10.1021/jp811257x

77 [Adsorption Configurations and Energies of Amino Acids on Anatase and Rutile Surfaces](#)

Koppen, S.; Bronkalla, O.; Langel, W.

J Phys Chem C (2008), 112(35), 13600-13606, DOI:10.1021/jp803354z

76 [Adsorption of small organic molecules on anatase and rutile surfaces: a theoretical study](#)

Koeppen, S.; Langel, W.

Phys Chem Chem Phys (2008), 10, 1907-1915. DOI:10.1039/b719098k

75 [Adsorption of collagen fragments on titanium oxide surfaces: a molecular dynamics study](#)

Koeppen, S.; Ohler, B.; Langel, W.

Z Phys Chem (2007), 221, 3-20. DOI:10.1524/zpch.2007.221.1.3

74 [Computer simulation of surfaces](#)

Langel, W.

Edited By: Rieth, M.; Schommers, W.

Handbook of Theoretical and Computational Nanotechnology (2006), 9, 55-108.

73 Book review: [Condensed matter physics. Crystals, liquids, liquid crystals, and polymers Strobl, Gert, 2004](#)
Langel, W.

J Sol State Electrochem (2006), 11, 437-438. DOI:10.1007/s10008-006-0143-x

72 [Calculation of the ligating strength of N-heterocyclic germylenes - extending the \$\pi\$ -acceptor range](#)

Kuehl, O; Lifson, K; Langel, W

Eur J Org Chem (2006), (10), 2336-2343, DOI:10.1002/ejoc.200500889

71 [Directed evolution of an esterase from Pseudomonas fluorescens yields a mutant with excellent enantioselectivity and activity for the kinetic resolution of a chiral building block](#)

Schmidt, M.; Hasenpusch, D.; Kaehler, M.; Kirchner, U.; Wiggenghorn, K.; Langel, W.; Bornscheuer, U. T.

ChemBioChem (2006), 7, 805-809, DOI:10.1002/cbic.200500546

70 [Simulation of the interface of \(100\) rutile with aqueous ionic solution](#)

Koepfen, S.; Langel, W.

Surf. Sci. (2006), 600, 2040-2050, DOI:10.1016/j.susc.2006.02.042

69 [Sulphur on rutile\(110\). A theoretical study](#)

Langel, W.

Surf. Sci. (2006), 600, 1884-1890, DOI:10.1016/j.susc.2006.01.056

68 Book review: [Theoretical surface sciences: a microscopic perspective, by Axel Groß](#)

Langel, W.

J Sol State Electrochem (2005), 9, 531-533, DOI:10.1007/s10008-004-0600-3

67 Book review: [Oxide surfaces \(Surfactant sciences series, vol. 103\) by James A. Wingrave](#)

Langel, W.

J Sol State Electrochem (2003), 7, 731-732, DOI:10.1007/s10008-003-0432-6

66 Book review: [Fundamentals of Semiconductors; Physics and Materials Properties by Peter Y. Yu, Manuel Cardona](#)

Langel, W.

J Sol State Electrochem (2003), 7, 729-730, DOI:10.1007/s10008-003-0431-7

65 [Simulation of the interface between titanium oxide and amino acids in solution by first principles MD](#)

Langel, W.; Menken, L.

Surf Sci (2003), 538, 1-9, DOI:10.1016/S0039-6028(03)00723-4

64 [Bisphosphino ureas: flexible ligands with rigid backbone](#)

Kuhl, O.; Langel, W.

Inorg Chem Comm (2003), 6, 74-77, DOI:10.1016/S1387-7003(02)00689-5

63 Book review: [Molecular Electronic-Structure Theory Edited by T. Helgaker, P. Jorgensen, J. Olsen, T. Helgaker](#)

Langel, W.

J Sol State Electrochem (2002), 6, 359-360, DOI:10.1007/s10008-001-0256-1

62 Book review: [Adsorption on Silica Surfaces \(Surfactant Science Series, Vol. 90\) Edited by E. Papirer](#)

Langel, W.

J Sol State Electrochem (2002), 6, 142, DOI:10.1007/s100080100203

61 Book review: [Karl-Heinz Meiwes-Broer \(ed\) Metal clusters at surfaces: structure, quantum properties, physical chemistry \(Springer Series in Cluster Physics\)](#)

Langel, W.

J Sol State Electrochem (2001), 6, 69-70, DOI:10.1007/s100080000172

60 [Car-Parrinello simulation of H₂O dissociation on rutile](#)

Langel, W.

Surf Sci (2002), 496, 141-150, DOI:10.1016/S0039-6028(01)01606-5

59 Book review: [H. Haken, H.C. Wolf \(Eds\) The Physics Of Atoms And Quanta. Introduction To Experiments And Theory, 6th Edn. \(Advanced Texts In Physics\)](#)

Langel, W.

J Sol State Electrochem (2001), 5, 568, DOI:10.1007/s100080100196

58 Book review: [Metal Clusters. Edited by W. Ekardt](#)

Langel, W.

J Sol State Electrochem (2001), 5, 227, DOI:10.1007/s100080000136

57 [Orientational ordering in methane condensates in mesoporous SiO₂ modifications at low temperatures](#)

Asmussen, B.; Balszunat, D.; Gutt, C.; Press, W.; Langel, W.; Coddens, G.; Kahn, R.

Journal de Physique IV: Proceedings (2000), 10(Pr7, International Workshop on Dynamics in Confinement, 2000), Pr7/137-Pr7/141, DOI:10.1051/jp4:2000727

56 [Dynamics of methane molecules in porous TiO₂](#)

Krasnov, I. A.; Asmussen, B.; Gutt, C.; Press, W.; Langel, W.; Ferrand, M.

J Phys: Cond Matt (2000), 12, 1613-1626, DOI:10.1088/0953-8984/12/8/304

55 [Dynamics of methane molecules in the mesopores of controlled-pore glass at low temperatures](#)

Gutt, C.; Asmussen, B.; Krasnov, I.; Press, W.; Langel, W.; Kahn, R.

Phys Rev B (1999), 59, 8607-8614

54 [X-ray diffraction study of CCl₄ crystallization in Vycor and silica gel mesopores](#)

Schaefer, B.; Langel, W.

Berichte der Bunsen-Gesellschaft (1998), 102, 1568-1572

53 [Inelastic neutron scattering from H₂ on vapor deposited CO₂](#)

Knipp, A.; Langel, W.; Mutka, H.; Knozinger, E.

Eur Phys J B: (1998), 3, 109-117, DOI:10.1007/s100510050289

52 [Multi-dimensional tunnelling: spectroscopy, modeling and isotope effects of ammonia adsorbed on the MgO{1 0 0} surface](#)

Prager, M.; Havighorst, M.; Buttner, H.; Langel, W.

Physica B (1998), 241-243, 262-268, DOI:10.1016/S0921-4526(97)00565-6

51 [QMS-controlled production of nanocrystalline metals by inert gas condensation in a flow system](#)

Daub, O.; Langel, W.; Reiner, C.; Kienle, L.
Ber. Bunsen-Ges. Phys. Chem. (1997), 101, 1753-1756

50 [Contrast x-ray powder diffraction of solid rare gas nanocrystals in silica gel mesopores](#)

Schaefer, B.; Balszunat, D.; Langel, W.; Asmussen, B.
Mol Phys (1996), 89, 1057-1070, DOI:10.1080/00268979609482523

49 [Rotational excitations of methane molecules in porous media](#)

Balszunat, D.; Asmussen, B.; Mueller, M.; Press, W.; Langel, W.; Coddens, G.; Ferrand, M.; Buettner, H.
Physica B (1996), 226(1-3, International Workshop on Quasielastic Neutron Scattering, International Workshop on Quantum Tunnelling of Atoms and Molecules in Solids, 1995), 185-188, DOI:10.1016/0921-4526(96)00299-2

48 [Car-Parrinello simulation of NH₃ adsorbed on the MgO\(100\) surface](#)

Langel, W.
Chem Phys Lett (1996), 259, 7-14, DOI:10.1016/0009-2614(96)00725-7

47 [Cu₂O quantum-dot particles prepared from nanostructured copper](#)

Kellersohn, A.; Knoezinger, E.; Langel, W. Giersig, M.
Adv Mat (1995), 7, 562-5

46 [Ab initio molecular dynamics of H₂O adsorbed on solid MgO](#)

Langel, W. Parrinello, M.
J Chem Phys (1995), 103, 3240-52, DOI:10.1063/1.470256

45 [Mixed carbon dioxide-krypton solids: a new diluted quadrupole system](#)

Langel, W., Fleger, H. W., Knoezinger, E., Schuller, W.
Ber. Bunsenges. Phys. Chem. (1995), 99, 940-50

44 [Neutron spectroscopy and Car-Parrinello simulation at adsorbates on magnesium oxide surfaces](#)

Langel, W.
J Mol Struct (1995), 349, 69-72, DOI:10.1016/0022-2860(95)08711-4

43 [Production of nanocrystalline copper in a flow system](#)

Becker, A.; Langel, W.; Knoezinger, E.
Z Phys Chem N F (1995), 188, 17-28

42 [Hydrolysis at stepped MgO surfaces](#)

Langel, W.; Parrinello, M.
Phys Rev Lett (1994), 73, 504-7, DOI:10.1103/PhysRevLett.73.504

41 [Low temperature powder diffraction on vapor deposited disordered solids](#)

Becker, A.; Fleger, H. W.; Knoezinger, E.; Langel, W.
Materials Science Forum (1993), 133-136 (Proceedings of the Second European Powder Diffraction Conference, 1992, Pt. 2), 933-8, DOI:10.4028/www.scientific.net/MSF.133-136.933

40 [Structure and morphology of gas phase deposited ice](#)

Langel, W.; Fleger, H. W.; Knoezinger, E.
Berichte der Bunsen-Gesellschaft (1994), 98(1), 81-91

39 [Low temperature powder diffraction on vapor deposited disordered solids](#)

Langel, W.; Becker, A.; Fleger, H.-W.; Knoezinger, E.
J Mol Struct (1993), 297, 407-13, DOI:10.1016/0022-2860(93)80196-3

38 [Methane rotation and the phase diagram of methane/xenon](#)

Prager, M.; Asmussen, B.; Langel, W.; Carlile, C. J.; Blank, H.
J Chem Phys (1993), 99, 2052-8, DOI:10.1063/1.465269

37 [Structure and morphology of gas-phase-deposited molecular nitrogen](#)

Becker, A.; Langel, W.; Maass, S.; Knoezinger, E.
J Phys Chem (1993), 97, 5525-9, DOI:10.1021/j100123a012

36 [Methane tunneling in disordered, solid argon-nitrogen phases](#)

Langel, W.; Prager, M.; Fleger, H. W.; Knoezinger, E.; Lauter, H. J.; Blank, H.; Carlile, C. J.
J Chem Phys (1993), 98, 4838-49, DOI:10.1063/1.464993

35 [Matrix and surface properties of gas-phase-deposited carbon dioxide](#)

Knoezinger, E.; Schuller, W.; Langel, W.
J Phys Chem (1993), 97, 927-31, DOI:10.1021/j100106a019

34 [Librational spectra of pure and carbon-tetrachloride-diluted acetone measured by neutron inelastic scattering](#)

Langel, W.; Prager, M.
Z Physik B (1992), 89(3), 279-84, DOI:10.1007/BF01318157

33 [Rotational tunnelling and ammonia sites in argon and nitrogen matrices](#)

Havighorst, M.; Prager, M.; Langel, W.
Physica B (1992), 180-181(Pt. B), 674-6, DOI:10.1016/0921-4526(92)90431-Q

32 [Inelastic neutron scattering from matrix isolated species](#)

Langel, W.
Spectrochimica Acta, A: (1992), 48A, 405-27, DOI:10.1016/0584-8539(92)80066-6

31 [Structure and dynamics in pure and doped rare-gas matrixes](#)

Knoezinger, E.; Schuller, W.; Langel, W.
Far. Disc. Chem. Soc. (1988), 86 (Spectrosc. Low Temp.), 285-93

30 [Rotational excitations of methane molecules in a nonequilibrium krypton matrix](#)

Prager, M.; Langel, W.
J Chem Phys (1989), 90, 5889-90, DOI:10.1063/1.456402

29 [From isolated HCN molecules to the crystal: Inelastic neutron scattering, far infrared spectroscopy, and normal coordinate analysis](#)

Langel, W.; Kollhoff, H.; Knoezinger, E.
J Chem Phys (1989), 90, 3430-42, DOI:10.1063/1.455852

28 [Adsorption of molecular hydrogen at high pressure and temperature on molybdenum and tungsten disulfides; observed by inelastic neutron scattering](#)

Jones, P. N.; Knoezinger, E.; Langel, W.; Moyes, R. B.; Tomkinson, J.
Surf Sci (1988), 207, 159-76, DOI:10.1016/0039-6028(88)90253-1

27 [Inelastic neutron scattering from liquid and solid hydrogen at high momentum transfer](#)

Langel, W.; Price, D. L.; Simmons, R. O.; Sokol, P. E.
Phys Rev B (1988), 38, 11275-83

26 [Disordered phases in vapor-deposited rare gases](#)

Langel, W.; Schuller, W.; Knoezinger, E.; Fleger, H. W.; Lauter, H. J.
J Chem Phys (1988), 89, 1741-2, DOI:10.1063/1.455119

25 [Structure and dynamics of solid carbon tetrachloride matrixes doped with acetonitrile](#)

Deiseroth, H. J.; Popp, S.; Kollhoff, H.; Langel, W.; Knoezinger, E.
J Mol Struct (1988), 174, 89-94, DOI:10.1016/0022-2860(88)80139-X

24 [Intermolecular interactions in condensed matter](#)

Knoezinger, E.; Hoffmann, P.; Huth, M.; Kollhoff, H.; Langel, W.; Schrems, O.; Schuller, W.
Mikrochimica Acta (1988), 3(1-6), 123-40

23 [Methane in vapor deposited argon: An inelastic neutron scattering study](#)

Prager, M.; Langel, W.
J Chem Phys (1988), 88, 7995-9, DOI:10.1063/1.454256

22 Neutron scattering and dynamics of small molecules in cryogenic matrixes

Langel, W.; Kollhoff, H.; Knoezinger, E.; Prager, M.
Ber. Bunsenges. Phys. Chem. (1987), 91, 1257-61

21 Rotational tunneling of matrix-isolated tetramethyl compounds

Langel, W.; Prager, M.; Schrems, O.; Knoezinger, E.
Springer Proceedings in Physics (1987), 17(Quantum Aspects Mol. Motions Solids), 93-7.

20 Momentum distribution of molecular hydrogen in the crystalline phase

Langel, W.
Studies in Physical and Theoretical Chemistry (1987), 46(Dyn. Mol. Cryst.), 589-92

19 From isolated molecules to condensed matter

Knoezinger, E.; Langel, W.; Kollhoff, H.
Studies in Physical and Theoretical Chemistry (1987), 46(Dyn. Mol. Cryst.), 583-7

18 Rotational tunnelling in matrix isolated molecules

Prager, M.; Langel, W.
Studies in Physical and Theoretical Chemistry (1987), 46(Dyn. Mol. Cryst.), 643-8

17 Neutron scattering, magnetization, and Moessbauer measurements on europium palladium silicide (EuPd₂Si₂) with enriched europium-153 isotopes

Holland-Moritz, E.; Braun, E.; Roden, B.; Perscheid, B.; Sampathkumaran, E. V.; Langel, W.
Phys Rev B (1987), 35, 3122-30

16 Intermolecular interaction in Sn(CH₃)₄: An inelastic neutron scattering study of matrix isolated molecules

Prager, M.; Langel, W.
J Chem Phys (1986), 85, 5279-85, DOI:10.1063/1.451670

15 Cluster formation of hydrogen cyanide in solid and liquid CCl₄ matrixes

Knoezinger, E.; Kollhoff, H.; Langel, W.
J Chem Phys (1986), 85, 4881-9, DOI:10.1063/1.451723

14 Single particle scattering and momentum distributions in solid hydrogen

Langel, W.
J Mol Struct (1986), 143, 1-4, DOI:10.1016/0022-2860(86)85190-0

13 Intermolecular interactions and dynamics of molecules and clusters isolated in solid argon and CCl₄ matrixes

Knoezinger, E.; Kollhoff, H.; Schrems, O.; Langel, W.
J Mol Struct (1986), 141, 399-404, DOI:10.1016/0022-2860(86)80356-8

12 Inelastic neutron scattering of H₂O isolated in solid argon

Langel, W.; Knoezinger, E.; Kollhoff, H.
Chem Phys Lett (1986), 124(1), 44-7, DOI:10.1016/0009-2614(86)85010-2

11 A cryostat insert for neutron scattering experiments on vapor deposited non-equilibrium samples

Langel, W.; Kollhoff, H.; Knoezinger, E.
J Physics E (1986), 19, 86-7, DOI:10.1088/0022-3735/19/1/018

10 Inelastic neutron scattering and far IR spectroscopy of acetonitrile in solid Ar and CCl₄ matrixes

Langel, W.; Kollhoff, H.; Knoezinger, E.
Ber. Bunsenges. Phys. Chem. (1985), 89, 927-35

9 Primary processes of electronically excited particles. IV. Relaxation of rotation distributions

Hack, W.; Langel, W.
Bericht - Max-Planck-Institut fuer Stroemungsforschung (1983), (13), 101 pp

8 Inelastic neutron scattering of hydrogen trapped in solid argon

Langel, W.
Revue de Physique Appliquee (1984), 19(9), 755-7, DOI:10.1051/rphysap:01984001909075500

7 Electronic excitation and quenching of thiocarbonyl (CS) formed in the argon fluoride laser photolysis of carbon disulfide

Dornhoefer, G.; Hack, W.; Langel, W.

J Phys Chem (1984), 88(14), 3060-9, DOI:10.1021/j150658a026

6 Photophysics of difluoromethylene ($\sim A^1B_1(0,6,0)$) excited by a krypton fluoride laser at 248 nm.

3. Direct measurements of 1B_1 collisional removal rates

Hack, W.; Langel, W.

J Phys Chem (1983), 87, 3462-8, DOI:10.1021/j100241a022

5 Photophysics of difluoromethylene (CF_2)($\sim A^1B_1(0,6,0)$) excited by a krypton fluoride laser at 248 nm.

2. Deactivation processes by inert gases

Dornhoefer, G.; Hack, W.; Langel, W.

J Phys Chem (1983), 87, 3456-62, DOI:10.1021/j100241a021

4 Photophysics of difluoromethylene ($\sim A^1B_1(0,6,0)$) excited by a krypton fluoride laser at 248 nm.

1: Quenching of difluoromethylene ($\sim A$) by its common precursors

Hack, W.; Langel, W.

J Photochem (1983), 21, 105-10, DOI:10.1016/0047-2670(83)80013-6

3 Noble gas halogen laser induced fluorescence of benzene, some of its derivatives, difluoromethyl radicals, and carbon monoxide

Langel, W.

Report (1980), (MPIS-22/1980), 124 pp

2 Formation of diatomic carbon ($e^3\Pi_g, C^1\Pi_g$) in the photolysis of carbon monoxide ($X^1\Sigma_g^+$) at 193 nm with an argon fluoride (ArF) laser

Hack, W.; Langel, W.

Chem Phys Lett (1981), 81, 387-90, DOI:10.1016/0009-2614(81)85635-7

1 Krypton fluoride (KrF) laser-induced fluorescence of benzene and its fluorinated derivatives in the gas phase

Hack, W.; Langel, W.

Nuovo Cimento della Societa Italiana di Fisica, B (1981), 63B, 207-20