

Prof. Dr. Volker Staemmler

**Liste der Veröffentlichungen
Stand August 2018**

1. V. Staemmler, W. Kutzelnigg
Die horizontale Korrelation in π -Elektronensystemen und ihre Beschreibung durch Elektronenpaarfunktionen.
Theoret. Chim. Acta 9, 67 (1967)
2. V. Dyczmons, V. Staemmler, W. Kutzelnigg
Near Hartree-Fock Energy and Equilibrium Geometry of CH_5^+ .
Chem. Phys. Letters 5, 361 (1970)
3. M. Gélus, R. Ahlrichs, V. Staemmler, W. Kutzelnigg
Origin of the Dimerization Energy of BH_3 to B_2H_6 .
Chem. Phys. Letters 7, 503 (1970)
4. M. Gélus, R. Ahlrichs, V. Staemmler, W. Kutzelnigg
Ab Initio Calculations of Small Hydrides Including Electron Correlation.
VI. Study of the Correlation Energy of the BH Ground State and Its Dependence on the Internuclear Distance.
Theoret. Chim. Acta 21, 63 (1971)
5. W. Kutzelnigg, V. Staemmler, M. Gélus
Potential Curve of the Lowest Triplet State of Li_2 .
Chem. Phys. Letters 13, 496 (1972)
6. V. Staemmler, M. Jungen
The Direct Determination of Brueckner Orbitals with Application to the H_2 Molecule.
Theoret. Chim. Acta 24, 152 (1972)
7. V. Staemmler, M. Jungen
Ab Initio Calculations of Small Hydrides Including Electron Correlation.
VII. The Two Lowest States of the BH_2 Radical.
Chem. Phys. Letters 16, 187 (1972)
8. W. Kutzelnigg, V. Staemmler, C. Hoheisel
Computed Potential Hypersurface (Including Electron Correlation) of the System Li^+/H_2 .
Chem. Phys. 1, 27 (1973)
9. F. Driessler, R. Ahlrichs, V. Staemmler, W. Kutzelnigg
Ab Initio Calculations on Small Hydrides Including Electron Correlation.
XI. Equilibrium Geometries and Other Properties of CH_3 , CH_3^+ , and CH_3^- , and Inversion Barrier of CH_3^- .
Theoret. Chim. Acta 30, 315 (1973)

10. V. Staemmler
Ab Initio Calculations on Small Hydrides Including Electron Correlation.
X. Triplet-Singlet Energy Separation and Other Properties of the CH₂ Radical.
Theoret. Chim. Acta 31, 49 (1973)
11. V. Staemmler
Ab Initio Calculation of the Lowest Singlet and Triplet States
in CH₂, CHF, CF₂, and CHCH₃.
Theoret. Chim. Acta 35, 309 (1974)
12. V. Staemmler
Ab Initio Calculation of the Potential Energy Surface of the System N₂Li⁺.
Chem. Phys. Z, 17 (1975)
13. R. Ahlrichs, H. Lischka, V. Staemmler, W. Kutzelnigg
PNO-CI (Pair Natural Orbital Configuration Interaction) and CEPA-PNO (Coupled
Electron Pair Approximation with Pair Natural Orbitals) Calculations of Molecular
Systems.
I. Outline of the Method for Closed Shell States.
J. Chem. Phys. 62, 1225 (1975)
14. R. Ahlrichs, F. Driessler, H. Lischka, V. Staemmler, W. Kutzelnigg
PNO-CI (Pair Natural Orbital Configuration Interaction) and CEPA-PNO (Coupled
Electron Pair Approximation with Pair Natural Orbitals) Calculations of Molecular
Systems.
II. The Molecules BeH₂, BH, BH₃, CH₄, CH₃⁻, NH₃ (Planar and Pyramidal), H₂O, OH₃⁺, HF
and the Ne Atom.
J. Chem. Phys. 62, 1235 (1975)
15. R. Ahlrichs, F. Keil, H. Lischka, W. Kutzelnigg, V. Staemmler
PNO-CI (Pair Natural Orbital Configuration Interaction) and CEPA-PNO (Coupled
Electron Pair Approximation with Pair Natural Orbitals) Calculations of Molecular
Systems.
III. The Molecules MgH₂, AlH₃, SiH₄, PH₃ (Planar and Pyramidal), H₂S, HCl and the Ar
Atom.
J. Chem. Phys. 63, 455 (1975)
16. V. Staemmler, M. Jungen
Application of the Independent Electron Pair Approach to the Calculation of Excitation
Energies, Ionization Potentials, and Electron Affinities of First Row Atoms.
Theoret. Chim. Acta 38, 303 (1975)
17. R. Ahlrichs, V. Staemmler
Ab Initio Study of the Electronic Structure of Diimide.
Chem. Phys. Letters 37, 77 (1976)
18. P. C. Hariharan, V. Staemmler
Potential Energy Curve of ¹Σ⁺ Li⁺/He.
Chem. Phys. 15, 409 (1976)

19. V. Staemmler
Ab Initio Calculation of the Potential Energy Surface of the System Li^+/CO .
Chem. Phys. 17, 187 (1976)
20. H. Kollmar, V. Staemmler
A Theoretical Study of the Structure of Cyclobutadiene.
J. Am. Chem. Soc. 99, 3583 (1977)
21. V. Staemmler
Note on Open Shell Restricted SCF Calculations for
Rotation Barriers about C-C Double Bonds: Ethylene and Allene.
Theoret. Chim. Acta 45, 89 (1977)
22. H. Kollmar, V. Staemmler
Violation of Hund's Rule by Spin Polarization in Molecules.
Theoret. Chim. Acta 48, 223 (1978)
23. H. Kollmar, V. Staemmler
On the Structure of Cyclobutadiene: Theoretical Determination of its Infrared Spectrum.
J. Am. Chem. Soc. 100, 4304 (1978)
24. M. Jungen, J. Vogt, V. Staemmler
Feshbach-Resonances and Dissociative Electron Attachment of H_2O .
Chem. Phys. 37, 49 (1979)
25. H. Kollmar, V. Staemmler
Ab Initio Calculations of the Potential Energy Surface of
the Reaction of Singlet Methylene with the Hydrogen Molecule.
Theoret. Chim. Acta 51, 207 (1979)
26. R. Jaquet, W. Kutzelnigg, V. Staemmler
Ab Initio Study, Including Electron Correlation, of the Electronic Structures,
the Dipole Moments, the Static Polarizabilities and of the Harmonic Force
Fields of H_2CO , H_2CS and H_2SiO .
Theoret. Chim. Acta 54, 205 (1980)
27. V. Staemmler, R. Jaquet
CEPA Calculations on Open-Shell Molecules.
I. Outline of the Method.
Theoret. Chim. Acta 59, 487 (1981)
28. V. Staemmler, R. Jaquet
CEPA Calculations on Open-Shell Molecules.
II. Singlet-Triplet Energy Splitting in π^2 Configurations of Diatomic Molecules.
Theoret. Chim. Acta 59, 501 (1981)

29. J. Wasilewski, V. Staemmler, R. Jaquet
CEPA Calculations on Open-Shell Molecules.
III. Potential Curves for the Six Lowest Excited States of He₂
in the Vicinity of their Equilibrium Distances.
Theoret. Chim. Acta 59, 517 (1981)
30. V. Staemmler, R. Jaquet, M. Jungen
CEPA Calculations on Open-Shell Molecules.
IV. Electron Correlation Effects in B₁-Rydberg States of H₂O.
J. Chem. Phys. 74, 1285 (1981)
31. R. Jaquet, V. Staemmler
CEPA Calculations of Potential Energy Surfaces for Open-Shell Systems.
I. The Reaction of O(³P) with H₂(¹Σ_g⁺)
Chem. Phys. 59, 373 (1981)
32. F. A. Gianturco, V. Staemmler
Selective Vibrational Inelasticity in Proton-Molecule Collisions.
In: B. Pullman (ed.), Intermolecular Forces, p. 79, Reidel 1981
(14. Jerusalem Symposium on Quantum Chemistry 1981)
33. P. Cársky, I. Hubac, V. Staemmler
Correlation Energies in Open-Shell Systems. Comparison of CEPA, PNO-CI and
Perturbation Treatments Based on Restricted Roothaan-Hartree-Fock Formalism.
Theoret. Chim. Acta 60, 445 (1982)
34. R. Jaquet, V. Staemmler
CEPA Calculations of Potential Energy Surfaces for Open-Shell Systems.
II. The Reaction of C⁺ Ions with Molecular Hydrogen.
Chem. Phys. 68, 479 (1982)
35. V. Staemmler
CEPA Calculations on Open-Shell Molecules.
V. The Vibration Frequencies of SF and SCl.
Theoret. Chim. Acta 62, 69 (1982)
36. V. Staemmler, R. Jaquet
CEPA Calculations for Rotation Barriers about CC Double Bonds: Ethylene, Allene, and
Methylene-Cyclopropane.
In: J. Hinze (ed.), Energy Storage and Redistribution in Molecules, p. 261, Plenum Press
1983
37. K. Kaufmann, M. Jungen, V. Staemmler
Can the H₅-Molecule be Observed?
Chem. Phys. 79, 111 (1983)

38. V. Staemmler
CEPA Calculations on Open-Shell Molecules.
VI. The First Ionization Potential of HCO.
Theoret. Chim. Acta 64, 205 (1983)
39. M. Jungen, V. Staemmler
Rydberg States of H₄.
Chem. Phys. Letters 103, 191 (1983)
40. W. W. Schoeller, V. Staemmler
Substituent Effects on Bonding Properties in Diphosphenes, Disilenes, and Diimines.
Inorg. Chem. 23, 3369 (1984)
41. V. Staemmler, R. Jaquet
CEPA Calculations of Potential Energy Surfaces for Open-Shell Systems.
III. Van der Waals Interaction Between O(³P) and He(¹S).
Chem. Phys. 92, 141 (1985)
42. V. Staemmler, A. Palma
CEPA Calculations of Potential Energy Surfaces
for Open-Shell Systems.
IV. Photodissociation of H₂O in the A¹B₁ State.
Chem. Phys. 93, 63 (1985)
43. B. Haug, H. Morgner, V. Staemmler
Experimental and Theoretical Study of Penning
Ionization of H₂O by Metastable Helium He(2³S).
J. Phys. B: At. Mol. Phys. 18, 259 (1985)
44. R. Schinke, V. Engel, V. Staemmler
Ab Initio Study of the Photodissociation of Water:
OH State Distributions and Comparison with Experiment.
Chem. Phys. Letters 116, 165 (1985)
45. U. Buck, K. H. Kohl, A. Kohlhase, M. Faubel, V. Staemmler
Rotationally Inelastic Scattering and Potential Calculations for He+CH₄.
Mol. Phys. 55, 1255 (1985)
46. R. Schinke, V. Engel, V. Staemmler
Rotational State Distributions in the Photolysis of Water:
Influence of the Potential Anisotropy.
J. Chem. Phys. 83, 4522 (1985)
47. V. Staemmler, F. A. Gianturco
Adiabatic SCF Potential Energy Curves Relevant to
Proton-Oxygen Molecular Collisions.
Int. J. Quantum Chem. 28, 553 (1985)

48. R. Jaquet, V. Staemmler
CEPA Calculations of Potential Energy Surfaces for Open-Shell Systems.
V. The O₂-He van der Waals Potential.
Chem. Phys. 101, 243 (1986)
49. F. A. Gianturco, A. Palma, E. Semprini, F. Stefani, H. P. Diehl,
V. Staemmler
Rotational Energy Transfers in Proton Collisions with CO₂ and HF Targets.
Chem. Phys. 107, 293 (1986)
50. V. Engel, R. Schinke, V. Staemmler
An Ab Initio Calculation of the Absorption Cross Section of
Water in the First Absorption Continuum.
Chem. Phys. Lett. 130, 413 (1986)
51. J. Wasilewski, V. Staemmler
CEPA Calculations on Open-Shell Molecules.
VII. Electronic Structure and Properties of HNS.
Inorg. Chem. 25, 4221 (1986)
52. W. W. Schoeller, V. Staemmler, P. Rademacher, E. Niecke
Theoretical Studies on Inorganic Ring Systems. Tetraphosphatricyclobutane,
Cyclotriphosphane, and White Phosphorus. Ring Strain and Hybridization.
Inorg. Chem. 25, 4382 (1986)
53. U. Meier, M. Schindler, V. Staemmler
Ein vektorisiertes Zweielektronenintegralprogramm.
in: H. Ehlich, K.-H. Schloßer, B. Wojcieszynski (eds.)
Proceedings of the 1985 Conferences on Supercomputers and
Applications, p. 209, Bochum 1986
54. V. Engel, R. Schinke, V. Staemmler
Photodissociation Dynamics of H₂O and D₂O in the First Absorption Band:
A Complete Ab Initio Treatment.
J. Chem. Phys. 88, 129 (1988)
55. M. Jungen, V. Staemmler
Potential Energy Curves for the Rydberg States of LiHe and the
spectrum of Li Atoms Interacting with He Gas.
J. Phys. B: At. Mol. Opt. Phys. 21, 463 (1988)
56. R. Schinke, V. Staemmler
Photodissociation Dynamics of H₂O₂ at 193 nm: An Example of the
Rotational Reflection Principle.
Chem. Phys. Lett. 145, 486 (1988)

57. J. Wasilewski, V. Staemmler, S. Koch
Coupled-Electron-Pair Approximation Calculations on Open-Shell Molecules: The Two Lowest States of HeNe⁺.
Phys. Rev. A 38, 1289 (1988)
58. V. Staemmler
CEPA Calculations on Open-Shell Molecules.
IX. Vertical Excitation Energies of Hydroxylamine and Hydrazine.
Acta Phys. Polon. A 74, 331 (1988)
59. J. Wasilewski, V. Staemmler
A Practical Double-Configuration (DC) SCF Algorithm
Based on a Complete Set of Generalized Brillouin Conditions.
Acta Phys. Polon. A 74, 355 (1988)
60. S. Henning, V. Engel, R. Schinke, V. Staemmler
Emission Spectroscopy of Photodissociating Water Molecules:
A Time-Independent ab initio Study
Chem. Phys. Lett. 149, 455 (1988)
61. H. R. Koslowski, B. A. Huber, V. Staemmler
Angular Distribution of Ar⁺ Ions Resulting from Single-Electron
Capture in Ar²⁺-He Collisions
J. Phys. B: At. Mol. Opt. Phys. 21, 2923 (1988)
62. U. Meier, V. Staemmler
An Efficient First-Order CASSCF Method Based on the Renormalized Fock-Operator
Technique.
Theoret. Chim. Acta 76, 95 (1989)
63. R. Jonas, V. Staemmler
CEPA Calculations of Potential Energy Surfaces for Open-Shell Systems.
VII. The 1³A' and 2³A'' states of NH(A³Π)-He.
Z. Phys. D 14, 143 (1989)
64. V. Staemmler
CEPA Calculations on Open-Shell Molecules.
XI. The Two Lowest Electronic States of HeAr⁺.
Z. Phys. D 16, 167 (1990)
65. V. Staemmler
Ab Initio Study of Small He Cluster Ions He_n⁺, n = 2,3,4,5,
and Low-Lying Rydberg States of He₄
Z. Phys. D 16, 219 (1990)

66. K. Weide, V. Staemmler, R. Schinke
Nonadiabatic Effects in the Photodissociation of H₂S.
J. Chem. Phys. 93, 861 (1990)
67. J. Urban, R. Jaquet, V. Staemmler
Theoretical Study of the Reaction Ne+H₂⁺ → NeH⁺ + H in the ²A' Ground State
Int. J. Quantum Chem. 38, 339 (1990)
68. H. Kühlenbeck, G. Odörfer, R. Jaeger, G. Illing, M. Menges, Th. Mull, H.-J. Freund,
M. Pöhlchen, V. Staemmler, S. Witzel, C. Scharfschwerdt, K. Wennemann, T. Liedtke,
M. Neumann
Molecular Adsorption on Oxide Surfaces: Electronic Structure and Orientation of NO on
NiO(100)/Ni(100) and on NiO(100) as Determined from Electron Spectroscopies and
ab-initio Cluster Calculations
Phys. Rev. B 43, 1969 (1991)
69. V. Staemmler, D. R. Flower
Excitation of the C(2p² ³P_J) Fine Structure States in Collisions with He(1s² ¹S₀)
J. Phys. B: At. Mol. Opt. Phys. 24, 2343 (1991)
70. K. Schröder, V. Staemmler, M. D. Smith, D. R. Flower, R. Jaquet
Excitation of the Fine-Structure Transitions of C in Collisions with Ortho- and Para-H₂
J. Phys. B: At. Mol. Opt. Phys. 24, 2487 (1991)
71. U. Meier, V. Staemmler
CASSCF and CEPA Calculations for the Photodissociation of HN₃.
II. Photodissociation into N₂ and NH on the Lowest ¹A' Surface of HN₃
J. Phys. Chem. 95, 6111 (1991)
72. J. Urban, V. Klimo, V. Staemmler, R. Jaquet
The Reaction Ne+H₂⁺ (v=0,1,2,3,4) → NeH⁺+H: 3D Potential
Energy Surface and Quasiclassical Trajectory Calculations
Z. Phys. D 21, 329 (1991)
73. H. R. Koslowski, H. Lebius, V. Staemmler, R. Fink, K. Wiesemann,
B. A. Huber
Collisions of Doubly Charged Nitrogen Molecules with Rare Gas Atoms
J. Phys. B: At. Mol. Opt. Phys. 24, 5023 (1991)
74. R. Jaquet, V. Staemmler, M. D. Smith, D. R. Flower
Excitation of the Fine-Structure Transitions of O(³P_J) in Collisions with Ortho- and Para-H₂
J. Phys. B: At. Mol. Opt. Phys. 25, 285 (1992)
75. V. Staemmler
Ab Initio Calculation of the Vertical Excitation Energies of Small Helium Cluster Ions
Z. Phys. D 22, 741 (1992)

76. V. Engel, V. Staemmler, R. L. Vander Wal, F. F. Crim, R. J. Sension, B. Hudson, P. Andresen, S. Hennig, K. Weide, R. Schinke
Photodissociation of Water in the First Absorption Band: A
Prototype for Dissociation on a Repulsive Potential Energy Surface
J. Phys. Chem. 96, 3201 (1992)
77. M. Pöhlchen, V. Staemmler
Ab initio Calculations for the Adsorption of Small Molecules on Metal Oxide Surfaces. I.
Cluster Calculations for Carbon Monoxide CO on Nickel Oxide NiO(100)
J. Chem. Phys. 97, 2583 (1992)
78. K. Hegemann, V. Staemmler, R. Fink
Quantum Chemical ab initio Calculations for Excited States of F IV
Z. Phys. D 27, 211 (1993)
79. A. Freitag, V. Staemmler, D. Cappus, C. A. Ventrice Jr.,
K. Al-Shamery, H. Kuhlenbeck, H.-J. Freund
Electronic Surface States of NiO(100)
Chem. Phys. Lett. 210, 10 (1993)
80. R. Fink, V. Staemmler
A Multi-Configuration Reference CEPA Method Based on Pair Natural Orbitals
Theoret. Chim. Acta 87, 129 (1993)
81. V. Staemmler
Quantum Chemical ab initio Calculations for the Adsorption of Small Molecules on
NiO(100)
in: H.-J. Freund, E. Umbach (Eds.): „Adsorption on Ordered Surfaces of Ionic Solids and
Thin Films“,
Springer Series in Surface Sciences, Vol. 33, p. 169, Springer, Berlin 1993
82. H. Schindler, R. Vogelsang, V. Staemmler, M. A. Siddiqi, P. Svejda
Ab initio Intermolecular Potentials of Methane, Nitrogen and Methane + Nitrogen and Their
Use in Monte Carlo Simulations of Fluids and Fluid Mixtures
Molec. Phys. 80, 1413 (1993)
83. J. Urban, V. Staemmler
Theoretical Study of the Lowest Potential Energy Surfaces for the Reaction $O(^3P) +$
 $HBr(X^1\Sigma^+) \rightarrow OH(X^2\Pi) + Br(^2P)$
Chem. Phys. 178, 279 (1993)
84. L. Neitsch, F. Stuhl, V. Staemmler
Comparison of Calculated and Measured Intensities of the $P_2(C^1\Sigma_u^+,$
 $v' = 11 \rightarrow X^1\Sigma_g^+, v'' = 3-32)$ Vibrational Sequence
J. Mol. Spectrosc. 163, 119 (1994)

85. P. Chaudhuri, F. Birkelbach, M. Winter, V. Staemmler, P. Fleischhauer, W. Haase, U. Flörke, H.-J. Haupt
A Novel Tetranuclear $[\text{Cr}^{\text{III}}_2 \text{Mn}^{\text{III}}_2(\mu_3\text{-O})_2]^{\text{8+}}$ Core with an $S_T=0$ Spin Ground State
J. Chem. Soc., Dalton Trans. 1994, 2313
86. H. Biehl, G. Schönnenbeck, F. Stuhl, V. Staemmler
The Vacuum-Ultraviolet Photodissociation of $\text{NH}_2(\text{X}^2\text{B}_1) \rightarrow \text{NH}(\text{A}^3\Pi)+\text{H}$
J. Chem. Phys. 101, 3811 (1994)
87. J. Freitag, V. Staemmler
Ab initio Calculations for the Adsorption of Small Molecules on Metal Oxide Surfaces. Part 3. Adsorption of H and CH_3 Radicals on NiO(100)
J. Elec. Spectr. Relat. Phenom. 69, 99 (1994)
88. H.-J. Freund, M. Baerns, H. Hamann, H. Kühlenbeck, H. Papp, V. Staemmler, H. Neddermeyer
Moleküle auf komplexen Festkörperoberflächen. Auf dem Weg zum Modellkatalysator.
Rubin 1/94, p. 24 (1994)
89. K. Al-Shamery, I. Beauport, B. Baumeister, T. Klüner, Th. Mull, M. Menges, C. Fischer, H.-J. Freund, P. Andresen, J. Freitag, V. Staemmler
State and Spatially Resolved Studies of UV-Laser Induced Desorption of Molecules from Oxide Surfaces
Proceedings of the SPIE'S OE/LASER '94 Conference 2125, 182 (1994)
90. K. Fink, R. Fink, V. Staemmler
Ab Initio Calculation of the Magnetic Exchange Coupling in Linear Oxo-Bridged Binuclear Complexes of Titanium (III), Vanadium (III), and Chromium (III)
Inorg. Chem. 33, 6219 (1994)
91. C. Wang, K. Fink, V. Staemmler
A Quantum Chemical ab initio Study of the Superexchange Coupling in Binuclear Oxygen-Bridged Ni(II) Complexes
Chem. Phys. 192, 25 (1995)
92. A. Freitag, Ch. van Wüllen, V. Staemmler
An ab initio Study of the Chemical Bond and the ^{129}Xe NMR Chemical Shifts in M^+-Xe compounds, $\text{M}=\text{Li, Na, K, Cu, Ag}$
Chem. Phys. 192, 267 (1995)
93. W. R. Roth, V. Staemmler, M. Neumann, C. Schmuck
Radikal-Stabilisierungsenergie - das MMEVBH-Kraftfeld
Liebig's Ann. 1995, 1061

94. M. Haßel, H. Kuhlenbeck, H.-J. Freund, S. Shi, A. Freitag, V. Staemmler, S. Lütkehoff, M. Neumann
Electronic Surface States of CoO(100): An Electron Energy Loss Study
Chem. Phys. Lett. 240, 205 (1995)
95. M. Bender, D. Ehrlich, I. N. Yakovkin, F. Rohr, M. Bäumer, H. Kuhlenbeck, H.-J. Freund, V. Staemmler
Structural Rearrangement and Surface Magnetism on Oxide Surfaces: A Temperature-Dependent Low-Energy Electron Diffraction - Electron Energy Loss Spectroscopy Study of Cr₂O₃(111)/Cr(110)
J. Phys.: Condens. Matter 7, 5289 (1995)
96. N. U. Zhanpeisov, V. Staemmler, M. Baerns
A Quantum-Chemical MINDO/3 Study of Methane and Oxygen Interactions with a Pure and a Modified Calcium Oxide Surface
J. Mol. Catal. A: Chem. 101, 51 (1995)
97. K. Fink, V. Staemmler
Ab initio Calculations of the van der Waals Interactions in One- and Two-Dimensional Infinite Periodic Systems
J. Chem. Phys. 103, 2603 (1995)
98. Shi Shou-heng, V. Staemmler
Electronic Structure and Absorption Spectrum of the CoF₆⁴⁻ Cluster Ion in Crystals of LiF and MgF₂ by ab initio Calculations
Chemical Journal of the Chinese Universities 16, 1602 (1995)
(chinesisch)
99. S. Shi, V. Staemmler
Ab initio Study of Local d-d-Excitations in Bulk CoO, at the CoO(100) Surface, and in Octahedral Co²⁺ Complexes
Phys. Rev. B 52, 12345 (1995)
100. C. Wang, K. Fink, V. Staemmler
An ab initio Study of the Geometry Dependence of the Magnetic Exchange Coupling in Oxo-Bridged Binuclear Chromium (III) Complexes
Chem. Phys. 201, 87 (1995)
101. V. Staemmler
Ab initio Calculations of Electronic Surface States of Transition Metal Oxides and of the Superexchange Coupling in Oxo-Bridged Transition Metal Complexes
in: N. Russo, D.R. Salahub (eds.) Metal-Ligand Interactions, NATO ASI Series, Series C, Vol. 474, p. 473, Kluwer Academic Publishers, Dordrecht 1996

102. M. A. Nygren, L. G. M. Pettersson, A. Freitag, V. Staemmler, D.H. Gay, A. L. Rohl
Theoretical Models of the Polar Cu₂O(100) Cu⁺-Terminated Surface
J. Phys. Chem. 100, 294 (1996)
103. A. Remscheid, B.A. Huber, M. Pykavyj, V. Staemmler, K. Wiesemann
Electron Capture and Dissociation of the N₂^{q+} Molecule in Slow Ar⁸⁺/N₂ Collisions
J. Phys. B: At. Mol. Opt. Phys. 29, 515 (1996)
104. H.-J. Freund, H. Kuhlenbeck, V. Staemmler
Oxide Surfaces
Rep. Prog. Phys. 59, 283 (1996)
105. J. Klinkmann, D. Cappus, K. Homann, T. Risse, A. Sandell,
T. Porwol, H.-J. Freund, K. Fink, R. Fink, V. Staemmler
Autoionization Spectroscopy of CO on Metal Oxide Surfaces
J. Elec. Spectr. Relat. Phenom. 77, 155 (1996)
106. T. Klüner, H.-J. Freund, J. Freitag, V. Staemmler
Laser-Induced Desorption of NO from NiO(100): Ab initio
Calculations of Potential Surfaces for Intermediate Excited States
J. Chem. Phys. 104, 10030 (1996)
107. W. Behmenburg, A. Makonnen, A. Kaiser, F. Rebenrost,
V. Staemmler, M. Jungen, G. Peach, A. Devdariani,
S. Tserkovnyi, A. Zagrebin, E. Czuchaj
Optical Transitions in Excited Alkali + Rare Gas Collision
Molecules and Related Interatomic Potentials: Li* + He
J. Phys. B: At. Mol. Opt. Phys. 29, 3891 (1996)
108. F. Rohr, M. Bäumer, H.-J. Freund, J. A. Mejias,
V. Staemmler, S. Müller, L. Hammer, K. Heinz
Strong Relaxations at the Cr₂O₃(0001) Surface as Determined via
Low-Energy Electron Diffraction and Molecular Dynamics Simulations
Surf. Sci. 372, L 291 (1997)
Erratum: Surf. Sci. 389, 391 (1997)
109. V. Staemmler
Accurate ab initio Determination of the van der Waals
Interaction in the X²Σ⁺ Ground State of LiHe
Z. Phys. D 39, 121 (1997)
110. Ch. Kolczewski, K. Fink, V. Staemmler, L. Neitsch
Ab initio Calculation of Potential Energy Surfaces for the
Three Lowest Triplet States (1³A'', 1³A', 2³A'') of PH(X,A)-He
J. Chem. Phys. 106, 7637 (1997)

111. T. Klüner, H.-J. Freund, J. Freitag, V. Staemmler
Laser Induced Desorption of NO from NiO(100):
Characterization of Potential Energy Surfaces of Excited States
J. Mol. Catal. A: Chem. 119, 155 (1997)
112. K. Fink, C. Wang, V. Staemmler
Ab initio Calculations of the Magnetic Exchange Coupling in
Sulfur-Bridged Binuclear Ni(II) Complexes
Int. J. Quantum Chem. 65, 633 (1997)
113. F. Rittner, R. Fink, B. Boddenberg, V. Staemmler
Adsorption of Nitrogen on Rutile (110): Ab Initio Cluster Calculations
Phys. Rev. B 57, 4160 (1998)
114. T. Klüner, H.-J. Freund, V. Staemmler, R. Kosloff
Theoretical Investigation of Laser Induced Desorption of
Small Molecules from Oxide Surface: A First Principles Study
Phys. Rev. Lett. 80, 5208 (1998)
115. G. Schönnenbeck, H. Biehl, F. Stuhl, U. Meier, V. Staemmler
VUV Photolysis of Hydrazoic Acid: Absorption and Fluorescence
Excitation Spectra
J. Chem. Phys. 109, 2210 (1998)
116. M. El-Batanouny, G. Murthy, C. R. Willis, S. Kais, V. Staemmler
Feasibility of Measuring Surface Electron Spin Dynamics by
Inelastic Scattering of Metastable Helium Atoms
Phys. Rev. B 58, 7391 (1998)
117. T. Klüner, S. Thiel, H.-J. Freund, V. Staemmler
The Vibrational Excitation of NO Desorbing from NiO(100) after
UV Laser Irradiation: Is NO⁻ a Possible Intermediate Species?
Chem. Phys. Lett. 294, 413 (1998)
118. T. Klüner, S. Thiel, H.-J. Freund, V. Staemmler
Laser-Induced Desorption of NO from NiO(100): Ab initio- and Wave Packet Calculations
Proceedings of the SPIE'S OE/LASER '98 Conference
3272, 177 (1998)
119. A. Haas, U. Fleischer, M. Mätschke, V. Staemmler
Darstellung, Charakterisierung, quantenchemische Berechnungen
und chemische Reaktionen von Schwefeldiimin, dessen Ag- und Tl-Salze
sowie TINSO
Z. anorg. allg. Chem. 625, 681 (1999)

120. F. Rittner, B. Boddenberg, R. F. Fink, V. Staemmler
Adsorption of Nitrogen on Rutile (110).
2. Construction of a Full Five-Dimensional Potential Energy Surface
Langmuir 15, 1449 (1999)
121. M. Marynowski, W. Franzen, M. El-Batanouny, V. Staemmler
Observation of an Extraordinary Antiferromagnetic Transition on the NiO(100) Surface
by Metastable Helium Atom Diffraction
Phys. Rev. B 60, 6053 (1999)
122. K. Fink, C. Wang, V. Staemmler
Superexchange and Spin-Orbit Coupling in Chlorine-Bridged
Binuclear Cobalt (II) Complexes
Inorg. Chem. 38, 3847 (1999)
123. J. A. Mejias, V. Staemmler, H.-J. Freund
Electronic States of the Cr₂O₃(0001) Surface from ab initio
Embedded Cluster Calculations
J. Phys.: Condens. Matter 11, 7881 (1999)
124. T. Klüner, S. Thiel, V. Staemmler
Ab Initio Calculation of Proton Scattering from He(1s2s, ¹S): A First-Principles
Wavepacket Study Beyond the Born-Oppenheimer Approximation
J. Phys. B: At. Mol. Opt. Phys. 32, 4931 (1999)
125. Ch. Kolczewski, K. Fink, V. Staemmler
Ab initio Calculation of the Magnetic Exchange Coupling in Linear Oxo-Bridged
Heterobinuclear Complexes of Titanium (III), Vanadium (III), and Chromium (III)
Int. J. Quantum Chem. 76, 137 (2000)
126. St. Hövel, C. Kolczewski, M. Wühn, J. Albers, K. Weiss, V. Staemmler, Ch. Wöll
Pyridine Adsorption on the Polar ZnO(0001) Surface: Zn Termination versus O Termination
J. Chem. Phys. 112, 3909 (2000)
127. J. Urban, P. Mach, J. Mášik, I. Hubač, V. Staemmler
Ground and Excited States of the Ne₃⁺ Molecule
Chem. Phys. 255, 15 (2000)
128. M. Pykavy, V. Staemmler, F. Rittner
Ab initio Cluster Calculations for the Adsorption of Small Molecules on Oxide Surfaces -
From Single Molecules to Monolayers
in: P. Entel and D.E. Wolf (Editors), "Structure and Dynamics of Heterogeneous Systems",
p. 3, World Scientific, Singapore 2000

129. W. Zhao, G. Kerner, M. Asscher, M. Wilde, K. Al-Shamery, H.-J. Freund, V. Staemmler, M. Wierzbowska
Interaction and Diffusion of Potassium on Cr₂O₃(0001)/Cr(110)
Phys. Rev. B 62, 7527 (2000)
130. T. Grycuk, W. Behmenburg, V. Staemmler
Quantum Calculation of the Excitation Spectra of Li*He Probing Interaction Potentials and Dipole Moments
J. Phys. B: At. Mol. Opt. Phys. 34, 245 (2001)
131. M. Pykavy, V. Staemmler, O. Seiferth, H.-J. Freund
Adsorption of CO on Cr₂O₃(0001)
Surf. Sci. 479, 11 (2001)
132. S. Thiel, M. Pykavy, T. Klüner, H.-J. Freund, R. Kosloff, V. Staemmler
Three-Dimensional *Ab Initio* Quantum Dynamics of the Photodesorption of CO from Cr₂O₃(0001): Stereodynamic Effects
Phys. Rev. Lett. 87, 077601 (2001)
133. C. Kolczewski, R. Püttner, O. Plashkevych, H. Agren, V. Staemmler, M. Martins, G. Snell, A. S. Schlachter, M. Sant'Anna, G. Kaindl, L. G. M. Pettersson
Detailed Study of Pyridine at the C 1s and N 1s Ionization Thresholds: The Influence of the Vibrational Fine Structure
J. Chem. Phys. 115, 6426 (2001)
134. S. Thiel, M. Pykavy, T. Klüner, H.-J. Freund, R. Kosloff, V. Staemmler
Rotational Alignment in the Photodesorption of CO from Cr₂O₃(0001): A Systematic Three-Dimensional *ab initio* Study
J. Chem. Phys. 116, 762 (2002)
135. W. Behmenburg, A. Kaiser, H. Bettermann, T. Grycuk, V. Staemmler
The Near UV Emission Spectra of the Li*He Excimers: Experimental and Theoretical Studies
J. Phys. B: At. Mol. Opt. Phys. 35, 747 (2002)
136. S. Reiß, H. Krumm, A. Niklewski, V. Staemmler, Ch. Wöll
The Adsorption of Acenes on Rutile TiO₂(110): A Multi-Technique Investigation
J. Chem. Phys. 116, 7704 (2002)
137. V. Staemmler, K. Fink
An *ab initio* Cluster Study of the Magnetic Properties of the CoO(001) Surface
Chem. Phys. 278, 79 (2002)
138. H. Winter, A. Mertens, R. Pfandzelter, V. Staemmler
Energy Transfer of keV Ne Atoms to the Lattice of a LiF(001) Surface under Channeling
Phys. Rev. A 66, 022902 (2002)

139. P. S. Bagus, V. Staemmler, Ch. Wöll
Exchangeliike Effects for Closed-Shell Adsorbates: Interface Dipole and Work Function
Phys. Rev. Lett. 89, 096104 (2002)
140. S. Shi, Ch. Shi, K. Fink, V. Staemmler
An ab initio Study of the Adsorption of CO on a Zn₄O₄ Cluster with Wurtzite-Like Structure
Chem. Phys. 287, 183 (2003)
141. V. Staemmler, K. Fink, B. Meyer, D. Marx, M. Kunat, U. Burghaus, S. Gil Girol, Ch. Wöll
Stabilization of Polar ZnO-Surfaces: Validating Microscopic Models by Using CO as a Probe Molecule
Phys. Rev. Lett. 90, 106102 (2003)
142. M. Taut, K. Pernal, J. Cioslowski, V. Staemmler
Three Electrons in a Harmonic Oscillator Potential: Pairs versus Single Particles
J. Chem. Phys. 118, 4861 (2003)
143. S. Lederer, A. Mertens, H. Winter, F. Aumayr, HP. Winter, V. Staemmler
Electronic Processes near Kinematic Threshold for Grazing Scattering of Fast Hydrogen Atoms from a LiF(001) Surface
Nucl. Instr. and Meth. B 203, 23 (2003)
144. N. Rößler, V. Staemmler
Ab initio Calculations for the 2s and 2p Core Level Binding Energies of Atomic Zn, Zn Metal, and Zn Containing Molecules
Phys. Chem. Chem. Phys. 5, 3580 (2003)
145. F. Wennmohs, V. Staemmler, M. Schindler
Theoretical Investigation of Weak Hydrogen Bonds to Sulfur
J. Chem. Phys. 119, 3208 (2003)
146. V. Staemmler, C. Wöll
Wie Moleküle an Oberflächen haften: Im chemischen Gang die Wände entlang
Rubin, Wissenschaftsmagazin der Ruhr-Universität Bochum, ChemieRubin, S. 38, 2003
147. S. Borowski, T. Klüner, H.-J. Freund, I. Klinkmann, K. Al-Shamery, M. Pykavy, V. Staemmler
Lateral Velocity Distributions in Laser Induced Desorption of CO from Cr₂O₃(0001): Experiment and Theory
Appl. Phys. A 78, 223 (2004)
148. T. Strunskus, O. Fuchs, L. Weinhardt, C. Heske, M. Guraya, M. Muhler, V. Staemmler, Ch. Wöll
The Valence Electronic Structure of Zinc Oxide Powders as Determined by X-ray Emission Spectroscopy: Variation of Electronic Structure with Particle Size
J. Electr. Spectrosc. Relat. Phenom. 134, 183 (2004)

149. G. Pacchioni, C. Di Valentin, D. Dominguez-Ariza, F. Illas, T. Bredow, T. Klüner, V. Staemmler
Bonding of NH₃, CO, and NO to NiO and Ni-doped MgO: A Problem for Density Functional Theory
J. Phys.: Condens. Matter 16, S2497 (2004)
150. V. Staemmler
The Cluster Approach for the Adsorption of Small Molecules on Oxide Surfaces
Top. Organomet. Chem. 12, 219 (2005)
151. K. von Haefen, A. Metzethin, S. Rudolph, V. Staemmler, M. Havenith
High Resolution Spectroscopy of NO in Helium Droplets: A Prototype for Open Shell Molecular Interactions in a Quantum Solvent
Phys. Rev. Lett. 95, 215301 (2005)
152. N. Rössler, K. Kotsis, V. Staemmler
Ab initio Calculations of the Zn 2s and 2p Core Level Binding Energies in Zn oxo Compounds and ZnO
Phys. Chem. Chem. Phys. 8, 697 (2006)
153. K. Kotsis, V. Staemmler
Ab initio Calculations of the O1s XPS Spectra of ZnO and Zn oxo Compounds
Phys. Chem. Chem. Phys. 8, 1490 (2006)
154. V. Staemmler
Introduction to Hartree-Fock and CI Methods
In: J. Grotendorst, S. Blügel, D. Marx (eds), „Computational Nanoscience: Do it Yourself“, NIC Series, Vol. 31, p. 1, Forschungszentrum Jülich 2006
- 155d Y. Wang, R Kováčik, B. Meyer, K. Kotsis, D. Stodt, V. Staemmler, H. Qiu, F. Traeger, D. Langenberg, M. Muhler, C. Wöll
CO₂-Aktivierung durch ZnO unter Bildung eines ungewöhnlichen dreizähnigen Oberflächencarbonats
Angew. Chem. 119, 5722 (2007)
- 155e. Y. Wang, R Kováčik, B. Meyer, K. Kotsis, D. Stodt, V. Staemmler, H. Qiu, F. Traeger, D. Langenberg, M. Muhler, C. Wöll
CO₂ Activation by ZnO through the Formation of an Unusual Tridentate Surface Carbonate
Angew. Chem. Int. Ed. 46, 5624 (2007)
156. R. Caputo, B. P. Prascher, V. Staemmler, P. S. Bagus, C. Wöll
Adsorption of Benzene on Coinage Metals: A Theoretical Analysis Using Wavefunction-Based Methods
J. Phys. Chem. A 111, 12778 (2007)

157. E. Schreiner, N. N. Nair, R. Pollet, V. Staemmler, D. Marx
Dynamical Magnetostructural Properties of *Anabaena* Ferredoxin
PNAS 104, 20725 (2007)
158. L. Hallmann, A. Bashir, T. Strunskus, R. Adelung, V. Staemmler, Ch. Wöll, F. Tuczek
Self-Assembled Monolayers of Benzylmercaptan and p-Cyanobenzylmercaptan on Au(111)
Surfaces: Structural and Spectroscopic Characterization
Langmuir 24, 5726 (2008)
159. V. Staemmler, P. Reinhardt, F. Allouti, M. E. Alikhani
A Theoretical Study of the Electronic Structure of the Co_2O_2 Molecule
Chem. Phys. 349, 83 (2008)
160. K. Kotsis, D. Stodt, V. Staemmler, R. Kováčik, B. Meyer, F. Traeger, D. Langenberg, Th.
Strunskus, M. Kunat, Ch. Wöll
 CO_2 Adlayers on the Mixed Terminated ZnO(10-10) Surface Studied by Helium Atom
Scattering, Photoelectron Spectroscopy and ab initio Electronic Structure Calculations
Z. Phys. Chem. 222, 891 (2008)
161. N. N. Nair, E. Schreiner, R. Pollet, V. Staemmler, D. Marx
Magnetostructural Dynamics with the Extended Broken Symmetry Formalism:
Antiferromagnetic [2Fe-2S] Complexes
J. Chem. Theory Comput. 4, 1174 (2008)
162. O. Yu. Khyzhun, T. Strunskus, Ch. Wöll, H. Gies, V. Staemmler
Comparison of the O $K\alpha$ X-ray Emission Bands in Micro- and Mesoporous Silica
Materials and in α -Quartz
J. Chem. Phys. 129, 084711 (2008)
163. P. Mach, J. Urban, V. Staemmler
Dissociative Electron Attachment to Methyl Chloride. A Quasi-Diatomic Potential
Curve for the Fragmentation of the Metastable CH_3Cl^- Anion
Chem. Phys. 356, 164 (2009)
164. W. Xu, J. Ma, D. Peng, W. Zou, W. Liu, V. Staemmler
Excited States of ReO_4^- : A Comprehensive Time-Dependent Relativistic Density Functional
Theory Study
Chem. Phys. 356, 219 (2009)
165. I. Schmitt, K. Fink, V. Staemmler
The Method of Local Increments for the Calculation of Adsorption Energies of Atoms and
Small Molecules on Solid Surfaces. Part I. A single Cu Atom on the Polar Surfaces of ZnO
Phys. Chem. Chem. Phys. 11, 11196 (2009)
166. N. N. Nair, J. Ribas-Arino, V. Staemmler, D. Marx
Magnetostructural Dynamics from Hubbard-U Corrected Spin-Projection: [2Fe-2S]
Complex in Ferredoxin
J. Chem. Theory Comput. 6, 569 (2010)

167. S. A. Fiethen, V. Staemmler, N. N. Nair, J. Ribas-Arino, E. Schreiner, 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 (2010)
168. Y. K. Gao, F. Traeger, K. Kotsis, V. Staemmler
A Theoretical Study of the XP and NEXAFS Spectra of Alanine: Gas Phase Molecule, Crystal,
and Adsorbate at the ZnO(10-10) Surface
Phys. Chem. Chem. Phys. **13**, 10709 (2011)
169. V. Staemmler
Method of Local Increments for the Calculation of Adsorption Energies of Atoms and Small
Molecules on Solid Surfaces. 2. CO/MgO(001)
J. Phys. Chem. A **115**, 7153 (2011)
170. Md. E. Ali, N. N. Nair, V. Staemmler, D. Marx
Constrained Spin-Density Dynamics of an Iron-Sulfur Complex: Ferredoxin Cofactor
J. Chem. Phys. **136**, 224101 (2012)
171. F. Uhl, V. Staemmler
Ab initio Calculation of Correlation Effects for the O1s Core Electron Binding Energy in MgO
J. Phys.: Condens. Matter **24**, 305501 (2012)
172. K. Fink, V. Staemmler
A Modified CAS-CI Approach for an Efficient Calculation of Magnetic Exchange Coupling
Constants
Mol. Phys. **111**, 2594-2605 (2013)
- 172a. V. Staemmler, Ch. Hättig, D. Marx
Editorial for the "Special Issue of Molecular Physics in Honour of Professor Kutzelnigg"
Mol. Phys. **111**, 2375-2376 (2013)
173. Md. E. Ali, V. Staemmler, F. Illas, P. M. Oppeneer
Designing the Redox-Driven Switching of Ferro- to Antiferromagnetic Couplings in
Organic Diradicals
J. Chem. Theory Comput. **9**, 5216-5220 (2013)
174. C. J. Nelin, F. Uhl, V. Staemmler, P. S. Bagus, Y. Fujimori, M. Sterrer, H. Kuhlenbeck, H.-J.
Freund
Surface Core Level Binding Energy Shifts for MgO(100)
Phys. Chem. Chem. Phys. **16**, 21953-21956 (2014)
175. Md. E. Ali, N. N. Nair, M. Retegan, F. Neese, V. Staemmler, D. Marx
The Iron-Sulfur Core in Rieske Proteins is not Symmetric
J. Biol. Inorg. Chem. **19**, 1287-1293 (2014)
176. Md. E. Ali, V. Staemmler, D. Marx
Magnetostructural Dynamics of Rieske versus Ferredoxin Iron-Sulfur Cofactors
Phys. Chem. Chem. Phys. **17**, 6289-6296 (2015)

177. H. Qiu, V. Staemmler, H. Kuhlenbeck, E. Bauer, H.-J. Freund
Weak Thermal Reduction of Biphasic Fe₂O₃(0001) Films Grown on Pt(111): Sub-Surface Fe²⁺ Formation
Surf. Sci. 641, 30-36 (2015)
178. Z. Wu, A. Płucienik, F. E. Feiten, M. Naschitzki, W. Wachsmann, S. Gewinner, W. Schöllkopf, V. Staemmler, H. Kuhlenbeck, H.-J. Freund
Vibrational Action Spectroscopy of Solids: New Surface-Sensitive Technique
Phys. Rev. Lett. 119, 136101/1-136101/5 (2017)
179. M. Böckers, R. Franke, V. Staemmler
A Heuristic Estimate of Molecular Correlation Energies Using Pair Correlation Energies of Localized Molecular Orbitals
submitted for publication
180. L. Warczinski, R. Franke, V. Staemmler
A Novel Approach for a Fast Estimation of Dynamic Electron Correlation Energies in Large Organic Molecules
submitted for publication
181. F. Uhl, V. Staemmler
An ab initio Study of the O1s and Mg1s, Mg2s, Mg2p Core Electron Binding Energies in Bulk MgO
submitted for publication
182. F. Uhl, V. Staemmler
A Quantum Chemical Cluster Study of the Antiferromagnetic Coupling in Rubidium Superoxide RbO₂
to be published