

**Prof. Dr. Volker Staemmler**

**Liste der Veröffentlichungen  
Stand Oktober 2010**

1. V. Staemmler, W. Kutzelnigg  
Die horizontale Korrelation in  $\pi$ -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  $\text{CH}_5^+$ .  
Chem. Phys. Letters 5, 361 (1970)
3. M. Gélus, R. Ahlrichs, V. Staemmler, W. Kutzelnigg  
Origin of the Dimerization Energy of  $\text{BH}_3$  to  $\text{B}_2\text{H}_6$ .  
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  $\text{Li}_2$ .  
Chem. Phys. Letters 13, 496 (1972)
6. V. Staemmler, M. Jungen  
The Direct Determination of Brueckner Orbitals with Application to the  $\text{H}_2$  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  $\text{BH}_2$  Radical.  
Chem. Phys. Letters 16, 187 (1972)
8. W. Kutzelnigg, V. Staemmler, C. Hoheisel  
Computed Potential Hypersurface (Including Electron Correlation) of the System  $\text{Li}^+/\text{H}_2$ .  
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  $\text{CH}_3$ ,  $\text{CH}_3^+$ , and  $\text{CH}_3^-$ , and Inversion Barrier of  $\text{CH}_3^-$ .  
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 CH<sub>2</sub> Radical.  
Theoret. Chim. Acta 31, 49 (1973)
11. V. Staemmler  
Ab Initio Calculation of the Lowest Singlet and Triplet States  
in CH<sub>2</sub>, CHF, CF<sub>2</sub>, and CHCH<sub>3</sub>.  
Theoret. Chim. Acta 35, 309 (1974)
12. V. Staemmler  
Ab Initio Calculation of the Potential Energy Surface of the System N<sub>2</sub>Li<sup>+</sup>.  
Chem. Phys. 7, 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 BeH<sub>2</sub>, BH, BH<sub>3</sub>, CH<sub>4</sub>, CH<sub>3</sub><sup>-</sup>, NH<sub>3</sub> (Planar and Pyramidal), H<sub>2</sub>O, OH<sub>3</sub><sup>+</sup>, 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 MgH<sub>2</sub>, AlH<sub>3</sub>, SiH<sub>4</sub>, PH<sub>3</sub> (Planar and Pyramidal), H<sub>2</sub>S, 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 <sup>1</sup>Σ<sup>+</sup> Li<sup>+</sup>/He.  
Chem. Phys. 15, 409 (1976)

19. V. Staemmler  
Ab Initio Calculation of the Potential Energy Surface of the System  $\text{Li}^+/\text{CO}$ .  
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  $\text{H}_2\text{O}$ .  
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  $\text{H}_2\text{CO}$ ,  $\text{H}_2\text{CS}$  and  $\text{H}_2\text{SiO}$ .  
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  $\pi^2$  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 He<sub>2</sub>  
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 B<sub>1</sub>-Rydberg States of H<sub>2</sub>O.  
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(<sup>3</sup>P) with H<sub>2</sub>(<sup>1</sup>Σ<sub>g</sub><sup>+</sup>)  
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<sup>+</sup> 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 SC1.  
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 H<sub>5</sub>-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 H<sub>4</sub>.  
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(<sup>3</sup>P) and He(<sup>1</sup>S).  
Chem. Phys. 92, 141 (1985)
42. V. Staemmler, A. Palma  
CEPA Calculations of Potential Energy Surfaces  
for Open-Shell Systems.  
IV. Photodissociation of H<sub>2</sub>O in the  $\tilde{A} \ ^1B_1$  State.  
Chem. Phys. 93, 63 (1985)
43. B. Haug, H. Morgner, V. Staemmler  
Experimental and Theoretical Study of Penning  
Ionization of H<sub>2</sub>O by Metastable Helium He(2<sup>3</sup>S).  
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+CH<sub>4</sub>.  
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 O<sub>2</sub>-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 CO<sub>2</sub> 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 H<sub>2</sub>O and D<sub>2</sub>O 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 H<sub>2</sub>O<sub>2</sub> 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<sup>+</sup>.  
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<sup>+</sup> Ions Resulting from Single-Electron  
Capture in Ar<sup>2+</sup>-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 1<sup>3</sup>A' and 2<sup>3</sup>A'' states of NH(A<sup>3</sup>Π)-He.  
Z. Phys. D 14, 143 (1989)
64. V. Staemmler  
CEPA Calculations on Open-Shell Molecules.  
XI. The Two Lowest Electronic States of HeAr<sup>+</sup>.  
Z. Phys. D 16, 167 (1990)
65. V. Staemmler  
Ab Initio Study of Small He Cluster Ions He<sub>n</sub><sup>+</sup>, n = 2,3,4,5,  
and Low-Lying Rydberg States of He<sub>4</sub>  
Z. Phys. D 16, 219 (1990)

66. K. Weide, V. Staemmler, R. Schinke  
Nonadiabatic Effects in the Photodissociation of H<sub>2</sub>S.  
J. Chem. Phys. 93, 861 (1990)
67. J. Urban, R. Jaquet, V. Staemmler  
Theoretical Study of the Reaction Ne+H<sub>2</sub><sup>+</sup> → NeH<sup>+</sup> + H in the <sup>2</sup>A' Ground State  
Int. J. Quantum Chem. 38, 339 (1990)
68. H. Kuhlenbeck, 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(2p<sup>2</sup> <sup>3</sup>P<sub>j</sub>) Fine Structure States in Collisions with He(1s<sup>2</sup> <sup>1</sup>S<sub>0</sub>)  
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-H<sub>2</sub>  
J. Phys. B: At. Mol. Opt. Phys. 24, 2487 (1991)
71. U. Meier, V. Staemmler  
CASSCF and CEPA Calculations for the Photodissociation of HN<sub>3</sub>.  
II. Photodissociation into N<sub>2</sub> and NH on the Lowest <sup>1</sup>A'' Surface of HN<sub>3</sub>  
J. Phys. Chem. 95, 6111 (1991)
72. J. Urban, V. Klimo, V. Staemmler, R. Jaquet  
The Reaction Ne+H<sub>2</sub><sup>+</sup> (v=0,1,2,3,4) → NeH<sup>+</sup>+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(<sup>3</sup>P<sub>j</sub>) in Collisions with Ortho- and Para-H<sub>2</sub>  
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. Kühlenbeck, 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  $[\text{Cr}^{\text{III}}_2 \text{Mn}^{\text{III}}_2(\mu_3\text{-O})_2]^{\delta+}$  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  $\text{NH}_2(\tilde{X}^2\text{B}_1) \rightarrow \text{NH}(\text{A}^3\Pi)+\text{H}$   
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  $\text{CH}_3$  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  $^{129}\text{Xe}$  NMR Chemical Shifts in  $\text{M}^+\text{-Xe}$  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  
Liebigs 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 Cr<sub>2</sub>O<sub>3</sub>(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 CoF<sub>6</sub><sup>4-</sup> Cluster Ion in Crystals of LiF and MgF<sub>2</sub> 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 Co<sup>2+</sup> 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 Cu<sub>2</sub>O(100) Cu<sup>+</sup>-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 N<sub>2</sub><sup>q+</sup> Molecule in Slow Ar<sup>8+</sup>/N<sub>2</sub> Collisions  
J. Phys. B: At. Mol. Opt. Phys. 29, 515 (1996)
104. H.-J. Freund, H. Kühlenbeck, 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<sup>\*</sup> + 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 Cr<sub>2</sub>O<sub>3</sub>(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 X<sup>2</sup>Σ<sup>+</sup> 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 (1<sup>3</sup>A'', 1<sup>3</sup>A', 2<sup>3</sup>A'') 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<sup>-</sup> 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 Cr<sub>2</sub>O<sub>3</sub>(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, <sup>1</sup>S): 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 Ne<sub>3</sub><sup>+</sup> 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  $\text{Cr}_2\text{O}_3(0001)/\text{Cr}(110)$   
Phys. Rev. B 62, 7527 (2000)
130. T. Grycuk, W. Behmenburg, V. Staemmler  
Quantum Calculation of the Excitation Spectra of  $\text{Li}^*\text{He}$  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  $\text{Cr}_2\text{O}_3(0001)$   
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  $\text{Cr}_2\text{O}_3(0001)$ : 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  $\text{Cr}_2\text{O}_3(0001)$ : 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  $\text{Li}^*\text{He}$  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  $\text{TiO}_2(110)$ : 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  $\text{CoO}(001)$  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  $\text{LiF}(001)$  Surface under Channeling  
Phys. Rev. A 66, 022902 (2002)

139. P. S. Bagus, V. Staemmler, Ch. Wöll  
Exchangelike 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 Zn<sub>4</sub>O<sub>4</sub> 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 Cr<sub>2</sub>O<sub>3</sub>(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 NH<sub>3</sub>, 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  
CO<sub>2</sub>-Aktivierung durch ZnO unter Bildung eines ungewöhnlichen dreizähligen 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  
CO<sub>2</sub> 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. Tuzek  
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  $\text{Co}_2\text{O}_2$  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  
 $\text{CO}_2$  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  $\alpha$ -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  $\text{CH}_3\text{Cl}^-$  Anion  
Chem. Phys. 356, 164 (2009)
164. W. Xu, J. Ma, D. Peng, W. Zou, W. Liu, V. Staemmler  
Excited States of  $\text{ReO}_4^-$ : 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  
to be published
169. V. Staemmler  
The Method of Local Increments for the Calculation of Adsorption Energies of Atoms and Small  
Molecules on Solid Surfaces. II. CO/MgO(001)  
to be published
170. M. Kuiper, M. Speldrich, H. Schilder, V. Staemmler, H. Lueken  
Magnetic Anisotropy of Dichlorobis( $\eta^5$ -cyclopentadienyl) Complexes of Vanadium, Niobium,  
and Tantalum  
to be published