

Publikationen Prof. Gotthard Seifert – 1976 bis 2016

Stand 20.10.2016

1. Raychev, D.; Guskova, O.; Seifert, G.; Sommer, J.-U., Conformational and electronic properties of small benzothiadiazole-cored oligomers with aryl flanking units: Thiophene versus Furan. *Computational Materials Science* **2016**, 126, 287–298.
2. Sandonas, L. M.; Teich, D.; Gutierrez, R.; Lorenz, T.; Pecchia, A.; Seifert, G.; Cuniberti, G., Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. *Journal of Physical Chemistry C* **2016**, 120, (33), 18841–49.
3. Karpov, Y.; Erdmann, T.; Raguzin, I.; Al-Husseini, M.; Binner, M.; Lappan, U.; Stamm, M.; Gerasimov, K. L.; Beryozkina, T.; Bakulev, V.; Anokhin, D. V.; Ivanov, D. A.; Günther, F.; Gemming, S.; Seifert, G.; Voit, B.; Pietro, R. D.; Kiriy, A., High Conductivity in Molecularly p-Doped Diketopyrrolopyrrole-Based Polymer: The Impact of a High Dopant Strength and Good Structural Order. *Advanced Materials* **2016**, 28, 6003-10.
4. Tranca, D. C.; Seifert, G., A First-Principles Study of Metal-Decorated Graphene Nanoribbons for Hydrogen Storage. *Zeitschrift für Physikalische Chemie* **2016**, 230, (1), 791–808.
5. Schwalbe, S.; Trepte, K.; Seifert, G.; Kortus, J., Screening for high-spin metal organic frameworks (MOFs): density functional theory study on DUT-8(M-1,M-2) (with M-i = V, ... ,Cu). *Physical Chemistry Chemical Physics* **2016**, 18, (11), 8075-8080.
6. Rodríguez-Hernández, F.; Tranca, D. C.; Szyja, B. M.; Santen, R. A. v.; Martínez-Mesa, A.; Uranga-Piña, L.; Seifert, G., Water Splitting on TiO₂-Based Electrochemical Cells: A Small Cluster Study. *Journal of Physical Chemistry C* **2016**, 120, 437–449.
7. Radovsky, G.; Popovitz-Biro, R.; Lorenz, T.; Joswig, J.-O.; Seifert, G.; Houben, L.; Dunin-Borkowski, R. E.; Tenne, R., Tubular structures from the LnS-TaS₂ (Ln = La, Ce, Nd, Ho, Er) and LaSe-TaSe₂ misfit layered compounds. *Journal of Materials Chemistry C* **2016**, 4, (1), 89-98.
8. Günther, F.; Gemming, S.; Seifert, G., Hopping-Based Charge Transfer in Diketopyrrolopyrrole-Based Donor–Acceptor Polymers: A Theoretical Study. *Journal of Physical Chemistry C* **2016**, 120, (18), 9581–9587.
9. Fediai, A.; Ryndyk, D. A.; Seifert, G.; Mothes, S.; Claus, M.; Schröter, M.; Cuniberti, G., Towards an optimal contact metal for CNTFETs. *Nanoscale* **2016**.
10. Warmbier, R.; Seifert, G.; Scholz, R.; Quandt, A., On the Theory of Charge Transfer Energies at Donor-Acceptor Interfaces in Solar Cells. *Third Southern African Solar Energy Conference (SASEC2015)* **2015**.
11. Trepte, K.; Schwalbe, S.; Seifert, G., Electronic and magnetic properties of DUT-8(Ni). *Phys. Chem. Chem. Phys.* **2015**, 17, (26), 17122-17129.
12. Ruck, M.; Seifert, G., Zukunftsziel „atomare Elektronik“ - Möglichkeiten durch die Miniaturisierung der elektronischen Welt. *labor&more* **2015**, 7, 38 - 43.
13. Quesnel, E.; Seifert, G.; al., e., Graphene-based technologies for energy applications, challenges and perspectives. *2D Materials* **2015**, 2, 030204
14. Kvashnin, D. G.; Sorokin, P. B.; Seifert, G.; Chernozatonskii, L. A., MoS₂ decoration by Mo-atoms and the MoS₂–Mo–graphene heterostructure: a theoretical study. *Phys. Chem. Chem. Phys.* **2015**, 17, (43), 28770-28773.
15. Klechikov, A.; Mercier, G.; Sharifi, T.; Baburin, I. A.; Seifert, G.; Talyzin, A. V., Hydrogen storage in high surface area graphene scaffolds. *ChemComm* **2015**.
16. Eisbein, E.; Joswig, J.-O.; Seifert, G., Enhanced proton-transfer activity in imidazole@MIL-53(Al) systems revealed by molecular-dynamics simulations. *Microporous and Mesoporous Materials* **2015**.

17. Craco, L.; Selli, D.; Seifert, G.; Leoni, S., Revealing the hidden correlated electronic structure of strained graphene. *Physical Review B* **2015**, 91, 205120.
18. Brent, J. R.; Lewis, D. J.; Lorenz, T.; Lewis, E. A.; Savjani, N.; Haigh, S. J.; Seifert, G.; Derby, B.; O'Brien, P., Tin(II) Sulfide (SnS) Nanosheets by Liquid-Phase Exfoliation of Herzenbergite: IV–VI Main Group Two-Dimensional Atomic Crystals. *Journal of the American Chemical Society* **2015**, 137, (39), 12689-12696.
19. Bon, V.; Pallmann, J.; Eisbein, E.; Hoffmann, H. C.; Senkovska, I.; Schwedler, I.; Schneemann, A.; Henke, S.; Wallacher, D.; Fischer, R. A.; Seifert, G.; Brunner, E.; Kaskel, S., Characteristics of flexibility in metal-organic framework solid solutions of composition $[Zn_2(BME-bdc)_x(DB-bdc)_{2-x}dabco]_n$: *In situ* powder X-ray diffraction, *in situ* NMR spectroscopy, and molecular dynamics simulations. *Microporous and Mesoporous Materials* **2015**.
20. Baburin, I. A.; Klechikov, A.; Mercier, G.; Talyzin, A.; Seifert, G., Hydrogen adsorption by perforated graphene. *International Journal of Hydrogen Energy* **2015**, 40, (20), 6594-6599.
21. Zhang, D.-B.; Seifert, G.; Chang, K., Strain-Induced Pseudomagnetic Fields in Twisted Graphene Nanoribbons. *Physical Review Letters* **2014**, 112, (9), 096805.
22. Wendumu, T. B.; Seifert, G.; Lorenz, T.; Joswig, J.-O.; Enyashin, A., Optical Properties of Triangular Molybdenum Disulfide Nanoflakes. *Journal of Physical Chemistry Letters* **2014**, 5, 3636.
23. Warmbier, R.; Quandt, A.; Seifert, G., Dielectric Properties of Selected Metal–Organic Frameworks. *Journal of Physical Chemistry C* **2014**, 118, 11799-11805.
24. Trolle, M. L.; Seifert, G.; Pedersen, T. G., Theory of excitonic second-harmonic generation in monolayer MoS₂. *Physical Review B* **2014**, 89, 235410.
25. Lorenz, T.; Joswig, J.-O.; Seifert, G., Two-dimensional and tubular structures of misfit compounds: Structural and electronic properties. *Beilstein Journal of Nanotechnology* **2014**, 5, 2171–2178.
26. Lorenz, T.; Joswig, J.-O.; Seifert, G., Stretching and breaking of monolayer MoS₂—an atomistic simulation *2D Materials* **2014**, 1.
27. Lorenz, T.; Joswig, J.-O.; Seifert, G., Combined SnS@SnS₂ double layers: charge transfer and electronic structure. *Semiconductor Science and Technology* **2014**, 29, (6).
28. Lorenz, T.; Ghorbani-Asl, M.; Joswig, J.-O.; Heine, T.; Seifert, G., Is MoS₂ a robust material for 2D electronics? . *Nanotechnology* **2014**, 25, 445201.
29. Kunze, T.; Posselt, M.; Gemming, S.; Seifert, G.; Konicek, A. R.; Carpick, R. W.; Pastewka, L.; Moseler, M., Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. *Tribology Letters* **2014**, 53, (1), 119-126.
30. Joswig, J.-O.; Lorenz, T.; Wendumu, T. B.; Gemming, S.; Seifert, G., Optics, Mechanics, and Energetics of Two-Dimensional MoS₂ Nanostructures from a Theoretical Perspective. *Accounts of Chemical Research* **2014**, 48, 48-55.
31. Joswig, J.-O.; Lorenz, T.; Seifert, G., Photoexcitation in Dimers of Coumarin and 6-Alkylcoumarins. *Zeitschrift für Physikalische Chemie* **2014**, 228, 243–251.
32. Götze, A.; Makowski, S.; Kunze, T.; Hübner, M.; Zellbeck, H.; Weihnacht, V.; Leson, A.; Beyer, E.; Joswig, J.-O.; Seifert, G.; Abrasonis, G.; Posselt, M.; Fassbender, J.; Möller, W.; Gemming, S.; Krause, M., Tetrahedral Amorphous Carbon Coatings for Friction Reduction of the Valve Train in Internal Combustion Engines. *Advanced Engineering Materials* **2014**, 16, (10), 1226–1233.
33. Elstner, M.; Seifert, G., Density functional tight binding. *Philosophical Transactions of the Royal Society A* **2014**, 372, 20120483.
34. Eisbein, E.; Joswig, J.-O.; Seifert, G., Proton Conduction in a MIL-53(Al) Metal–Organic Framework: Confinement versus Host/Guest Interaction. *Journal of Physical Chemistry C* **2014**, 118, (24), 13035-13041.
35. Claus, M.; Teich, D.; Mothes, S.; Seifert, G.; Schröter, M., Impact of functionalization patterns on the performance of CNTFETs. *IWCE 2014* **2014**.

36. Brüser, V.; Popovitz-Biro, R.; Albu-Yaron, A.; Lorenz, T.; Seifert, G.; Tenne, R.; Zak, A., Single- to Triple-Wall WS₂ Nanotubes Obtained by High-Power Plasma Ablation of WS₂ Multiwall Nanotubes. *Inorganics* **2014**, 2, (2), 177-190.
37. Tayran, C.; Zhu, Z.; Baldoni, M.; Selli, D.; Seifert, G.; Tomanek, D., Optimizing Electronic Structure and Quantum Transport at the Graphene-Si(111) Interface: An Ab Initio Density-Functional Study. *Physical Review Letters* **2013**, 110, (17), 176805.
38. Sun, Q.-C.; Yadgarov, L.; Rosentsveig, R.; Seifert, G.; Tenne, R.; Musfeldt, J. L., Observation of a Burstein-Moss Shift in Rhenium-Doped MoS₂ Nanoparticles. *ACS nano* **2013**, 7, (4), 3506-11.
39. Selli, D.; Baburin, I.; Leoni, S.; Zhu, Z.; Tománek, D.; Seifert, G., Theoretical investigation of the electronic structure and quantum transport in the graphene-C(111) diamond surface system. *Journal of Physics: Condensed Matter* **2013**, 25, (43), 435302.
40. Scholz, R.; Luschtinetz, R.; Seifert, G.; Jägeler-Hoheisel, T.; Körner, C.; Leo, K.; Rapacioli, M., Quantifying charge transfer energies at donor-acceptor interfaces in small-molecule solar cells with constrained DFTB and spectroscopic methods. *Journal of Physics: Condensed Matter* **2013**, 25, (47), 473201-221.
41. Mondal, S. S.; Bhunia, A.; Baburin, I. A.; Jager, C.; Kelling, A.; Schilde, U.; Seifert, G.; Janiak, C.; Holdt, H.-J., Gate effects in a hexagonal zinc-imidazolate-4-amide-5-imidate framework with flexible methoxy substituents and CO₂ selectivity. *Chemical communications (Cambridge, England)* **2013**, 49, (69), 7599-601.
42. Luschtinetz, R.; Seifert, G., Theoretical studies on the structural and electronic properties of π -stacked cyano-thiophene-based molecules. *Computational and Theoretical Chemistry* **2013**, 1023, 65-73.
43. Luschtinetz, R.; Gemming, S.; Seifert, G., Theoretical study on the CH...NC hydrogen bond interaction in thiophene-based molecules. *Computational and Theoretical Chemistry* **2013**, 1005, 45-52.
44. Joswig, J.-O.; Lorenz, T.; Seifert, G., The Virtues of Magnetism. *ACS Nano* **2013**, 7, (12), 10449-10451.
45. Ghorbani-Asl, M.; Enyashin, A. N.; Kuc, A.; Seifert, G.; Heine, T., Defect-induced conductivity anisotropy in MoS₂ monolayers. *Physical Review B* **2013**, 88, 245440
46. Fthenakis, Z. G.; Zhu, Z.; Teich, D.; Seifert, G.; Tománek, D., Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. *Physical Review B* **2013**, 88, (24), 245402.
47. Fischer, M.; Handt, J.; Seifert, G.; Schmidt, R., Orientation dependence of energy absorption and relaxation dynamics of C₆₀ in fs-laser pulses. *Physical Review A* **2013**, 88, (6), 061403.
48. Enyashin, A. N.; Bar-Sadan, M.; Houben, L.; Seifert, G., Line Defects in Molybdenum Disulfide Layers. *Journal of Physical Chemistry C* **2013**, 117, (20), 10842-10848.
49. Baldoni, M.; Craco, L.; Seifert, G.; Leoni, S., A two-electron mechanism of lithium insertion into layered alpha-MoO₃: a DFT and DFT+U study. *Journal of Materials Chemistry A* **2013**, 1, (5), 1778-1784.
50. Yurchenko, S.; Seifert, G.; Lavrov, E. V.; Assfour, B., Combined IR absorption and modeling study of nanoporous Zeolite Imidazolate Frameworks (ZIFs) filled with hydrogen. *RSC Advances* **2012**, 2, (26), 9839-9845.
51. Yadgarov, L.; Rosentsveig, R.; Leitius, G.; Albu-Yaron, A.; Moshkovich, A.; Perfilyev, V.; Vasic, R.; Frenkel, A. I.; Enyashin, A. N.; Seifert, G.; Rapoport, L.; Tenne, R., Controlled Doping of MS₂ (M=W, Mo) Nanotubes and Fullerene-like Nanoparticles. *Angewandte Chemie-International Edition* **2012**, 51, (5), 1148-1151.
52. Teich, D.; Seifert, G.; Iijima, S.; Tománek, D., Helicity in Ropes of Chiral Nanotubes: Calculations and Observation. *Physical Review Letters* **2012**, 108, (23), 235501.

53. Teich, D.; Fthenakis, Z. G.; Seifert, G.; Tomanek, D., Nanomechanical Energy Storage in Twisted Nanotube Ropes. *Physical Review Letters* **2012**, 109, (25), 255501.
54. Selli, D.; Boulfelfel, S. E.; Baburin, I. A.; Seifert, G.; Leoni, S., Framework reconstruction between hR8 and cI16 germaniums: A molecular dynamics study. *RSC Advances* **2012**, 2, (23), 8833-8839.
55. Seifert, G.; Joswig, J.-O., Density-functional tight binding—an approximate density-functional theory method. *Wiley Interdisciplinary Reviews: Computational Molecular Science* **2012**, 2, (3), 456-465.
56. Popov, I.; Seifert, G.; Tománek, D., Designing Electrical Contacts to MoS₂ Monolayers: A Computational Study. *Physical Review Letters* **2012**, 108, (15), 156802.
57. Martinez-Mesa, A.; Zhechkov, L.; Yurchenko, S. N.; Heine, T.; Seifert, G.; Rubayo-Soneira, J., Hydrogen Physisorption on Carbon Foams upon Inclusion of Many-Body and Quantum Delocalization Effects. *Journal of Physical Chemistry C* **2012**, 116, (36), 19543-19553.
58. Manzano, H.; Enyashin, A. N.; Dolado, J. S.; Ayuela, A.; Frenzel, J.; Seifert, G., Do Cement Nanotubes exist? *Advanced Materials* **2012**, 24, (24), 3239-3245.
59. Lukose, B.; Supronowicz, B.; St Petkov, P.; Frenzel, J.; Kuc, A. B.; Seifert, G.; Vayssilov, G. N.; Heine, T., Structural properties of metal-organic frameworks within the density-functional based tight-binding method. *Physica Status Solidi B-Basic Solid State Physics* **2012**, 249, (2), 335-342.
60. Lorenz, T.; Teich, D.; Joswig, J.-O.; Seifert, G., Theoretical Study of the Mechanical Behavior of Individual TiS₂ and MoS₂ Nanotubes. *The Journal of Physical Chemistry C* **2012**, 116, (21), 11714-11721.
61. Leoni, S.; Baldoni, M.; Craco, L.; Joswig, J.-O.; Seifert, G., Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. *Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics* **2012**, 226, (2), 95-106.
62. Erdogan, E.; Popov, I. H.; Enyashin, A. N.; Seifert, G., Transport properties of MoS₂ nanoribbons: edge priority. *European Physical Journal B* **2012**, 85, (1), 33.
63. Enyashin, A. N.; Seifert, G., Density-functional study of Li_xMoS₂ intercalates (0 ≤ x ≤ 1). *Computational and Theoretical Chemistry* **2012**, 999, 13-20.
64. Debatin, F.; Behrens, K.; Weber, J.; Baburin, I. A.; Thomas, A.; Schmidt, J.; Senkovska, I.; Kaskel, S.; Kelling, A.; Hedin, N.; Bacsik, Z.; Leoni, S.; Seifert, G.; Jaeger, C.; Guenter, C.; Schilde, U.; Friedrich, A.; Holdt, H.-J., An Isorecticular Family of Microporous Metal-Organic Frameworks Based on Zinc and 2-Substituted Imidazolate-4-amide-5-imidate: Syntheses, Structures and Properties. *Chemistry-a European Journal* **2012**, 18, (37), 11630-11640.
65. Boulfelfel, S. E.; Seifert, G.; Grin, Y.; Leoni, S., Squeezing lone pairs: The A17 to A7 pressure-induced phase transition in black phosphorus. *Physical Review B* **2012**, 85, (1), 014110.
66. Teich, D.; Lorenz, T.; Joswig, J.-O.; Seifert, G.; Zhang, D.-B.; Dumitrică, T., Structural and Electronic Properties of Helical TiS₂ Nanotubes Studied with Objective Molecular Dynamics. *The Journal of Physical Chemistry C* **2011**, 115, (14), 6392-6396.
67. Radovsky, G.; Popovitz-Biro, R.; Staiger, M.; Gartsman, K.; Thomsen, C.; Lorenz, T.; Seifert, G.; Tenne, R., Synthesis of Copious Amounts of SnS₂ and SnS₂/SnS Nanotubes with Ordered Superstructures. *Angewandte Chemie International Edition* **2011**, 50, (51), 12316-12320.
68. Oliveira, A. F.; Gemming, S.; Seifert, G., Conformational Analysis of Aqueous BMP-2 Using Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B* **2011**, 115, (5), 1122-1130.
69. Martinez-Mesa, A.; Yurchenko, S. N.; Patchkovskii, S.; Heine, T.; Seifert, G., Influence of quantum effects on the physisorption of molecular hydrogen in model carbon foams. *The Journal of Chemical Physics* **2011**, 135, (21), 214701-9.
70. Lushtinetz, R.; Gemming, S.; Seifert, G., Anchoring functional molecules on TiO₂ surfaces: A comparison between the carboxylic and the phosphonic acid group. *The European Physical Journal Plus* **2011**, 126, (10), 1-13.

71. Kunze, T.; Gemming, S.; Posselt, M.; Seifert, G., Tribological Aspects of Carbon-Based Nanocoatings – Theory and Simulation. *Zeitschrift für Physikalische Chemie* **2011**, 225, (3), 379-387.
72. Krause, M.; Mücklich, A.; Zak, A.; Seifert, G.; Gemming, S., High resolution TEM study of WS₂ nanotubes. *physica status solidi (b)* **2011**, 248, (11), 2716-2719.
73. Kalfon-Cohen, E.; Goldbart, O.; Schreiber, R.; Cohen, S. R.; Barlam, D.; Lorenz, T.; Joswig, J. O.; Seifert, G., Experimental, finite element, and density-functional theory study of inorganic nanotube compression. *Applied Physics Letters* **2011**, 98, (8), 081908.
74. Kalfon-Cohen, E.; Goldbart, O.; Schreiber, R.; Cohen, S. R.; Barlam, D.; Lorenz, T.; Enyashin, A.; Seifert, G., Radial compression studies of WS₂ nanotubes in the elastic regime. *Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures* **2011**, 29, (2), 021009-021009-8.
75. Hoffmann, H. C.; Assfour, B.; Epperlein, F.; Klein, N.; Paasch, S.; Senkovska, I.; Kaskel, S.; Seifert, G.; Brunner, E., High-Pressure in Situ Xe-129 NMR Spectroscopy and Computer Simulations of Breathing Transitions in the Metal-Organic Framework Ni-2(2,6-ndc)(2)(dabco) (DUT-8(Ni)). *Journal of the American Chemical Society* **2011**, 133, (22), 8681-8690.
76. Frenzel, J.; Thieme, S.; Seifert, G.; Joswig, J.-O., Optical Excitations in CdSe/CdS Core-Shell Nanoparticles. *The Journal of Physical Chemistry C* **2011**, 115, (21), 10338-10344.
77. Erdogan, E.; Popov, I.; Seifert, G., Robust electronic and transport properties of graphene break nanojunctions. *Physical Review B* **2011**, 83, (24), 245417.
78. Erdogan, E.; Popov, I.; Rocha, C. G.; Cuniberti, G.; Roche, S.; Seifert, G., Engineering carbon chains from mechanically stretched graphene-based materials. *Physical Review B* **2011**, 83, (4), 041401.
79. Enyashin, A. N.; Yadgarov, L.; Houben, L.; Popov, I.; Weidenbach, M.; Tenne, R.; Bar-Sadan, M.; Seifert, G., New Route for Stabilization of 1T-WS₂ and MoS₂ Phases. *The Journal of Physical Chemistry C* **2011**, 115, (50), 24586-24591.
80. Boulfelfel, S. E.; Seifert, G.; Leoni, S., Atomistic investigation of Li⁺ diffusion pathways in the olivine LiFePO₄ cathode material. *Journal of Materials Chemistry* **2011**, 21, (41), 16365-16372.
81. Baburin, I. A.; Assfour, B.; Seifert, G.; Leoni, S., Polymorphs of lithium-boron imidazolates: energy landscape and hydrogen storage properties. *Dalton Transactions* **2011**, 40, (15), 3796-3798.
82. Assfour, B.; Leoni, S.; Yurchenko, S.; Seifert, G., Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. *International Journal of Hydrogen Energy* **2011**, 36, (10), 6005-6013.
83. Assfour, B.; Leoni, S.; Seifert, G.; Baburin, I. A., Packings of Carbon Nanotubes - New Materials for Hydrogen Storage. *Advanced Materials* **2011**, 23, (10), 1237-1241.
84. Albu-Yaron, A.; Levy, M.; Tenne, R.; Popovitz-Biro, R.; Weidenbach, M.; Bar-Sadan, M.; Houben, L.; Enyashin, A. N.; Seifert, G.; Feuermann, D.; Katz, E. A.; Gordon, J. M., MoS₂ Hybrid Nanostructures: From Octahedral to Quasi-Spherical Shells within Individual Nanoparticles. *Angewandte Chemie-International Edition* **2011**, 50, (8), 1810-1814.
85. Zhang, D.-B.; Dumitrica, T.; Seifert, G., Helical Nanotube Structures of MoS₂ with Intrinsic Twisting: An Objective Molecular Dynamics Study. *Physical Review Letters* **2010**, 104, (6), 065502.
86. Zagorodniy, K.; Seifert, G.; Hermann, H., Metal-organic frameworks as promising candidates for future ultralow-k dielectrics. *Applied Physics Letters* **2010**, 97, (25), 251905-2.
87. Xiao, R.; Fritsch, D.; Kuz'min, M. D.; Koepernik, K.; Richter, M.; Vietze, K.; Seifert, G., Prediction of huge magnetic anisotropies of transition-metal dimer-benzene complexes from density functional theory calculations. *Physical Review B* **2010**, 82, (20), 205125.
88. Wunderlich, F.; Leisegang, T.; Weissbach, T.; Zschornak, M.; Stoecker, H.; Dshemuchadse, J.; Lubk, A.; Fuehrlich, T.; Welter, E.; Souptel, D.; Gemming, S.; Seifert, G.; Meyer, D. C., EXAFS,

- XANES, and DFT study of the mixed-valence compound YMn₂O₅: Site-selective substitution of Fe for Mn. *Physical Review B* **2010**, 82, (1), 014409
89. Rasche, B.; Seifert, G.; Enyashin, A., Stability and Electronic Properties of Bismuth Nanotubes. *The Journal of Physical Chemistry C* **2010**, 114, (50), 22092-22097.
 90. Oliveira, A. F.; Gemming, S.; Seifert, G., Molecular dynamics simulations of BMP-2 adsorption on a hydrophobic surface. *Materialwissenschaft Und Werkstofftechnik* **2010**, 41, (12), 1048-1053.
 91. Milek, T.; Duchstein, P.; Seifert, G.; Zahn, D., Motif Reconstruction in Clusters and Layers: Benchmarks for the Kawska-Zahn Approach to Model Crystal Formation. *ChemPhysChem* **2010**, 11, (4), 847-852.
 92. Luschtinetz, R.; Oliveira, A. F.; Duarte, H. A.; Seifert, G., Self-assembled Mono layers of Alkylphosphonic Acids on Aluminum Oxide Surfaces - A Theoretical Study. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2010**, 636, (8), 1506-1512.
 93. Levi, R.; Bar-Sadan, M.; Albu-Yaron, A.; Popovitz-Biro, R.; Houben, L.; Shahar, C.; Enyashin, A.; Seifert, G.; Prior, Y.; Tenne, R., Hollow V₂O₅ Nanoparticles (Fullerene-Like Analogues) Prepared by Laser Ablation. *Journal of the American Chemical Society* **2010**, 132, (32), 11214-11222.
 94. Kunze, T.; Gemming, S.; Pankoke, V.; Morawetz, K.; Luschtinetz, R.; Seifert, G., Electronic transport properties through thiophenes on switchable domains. *Physical Review B* **2010**, 81, (11), 115401.
 95. Kuc, A.; Heine, T.; Seifert, G., Structural and electronic properties of graphene nanoflakes. *Physical Review B* **2010**, 81, (8), 085430.
 96. Kreizman, R.; Enyashin, A. N.; Deepak, F. L.; Albu-Yaron, A.; Popovitz-Biro, R.; Seifert, G.; Tenne, R., Synthesis of Core-Shell Inorganic Nanotubes. *Advanced Functional Materials* **2010**, 20, (15), 2459-2468.
 97. Khvostikova, O.; Assfour, B.; Seifert, G.; Hermann, H.; Horst, A.; Ehrenberg, H., Novel experimental methods for assessment of hydrogen storage capacity and modelling of sorption in Cu-BTC. *International Journal of Hydrogen Energy* **2010**, 35, (20), 11042-11051.
 98. Hong, S. Y.; Kreizman, R.; Rosentsveig, R.; Zak, A.; Sloan, J.; Enyashin, A. N.; Seifert, G.; Green, M. L. H.; Tenne, R., One- and Two-Dimensional Inorganic Crystals inside Inorganic Nanotubes. *European Journal of Inorganic Chemistry* **2010**, (27), 4233-4243.
 99. Guimaraes, L.; Enyashin, A. N.; Seifert, G.; Duarte, H. A., Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. *Journal of Physical Chemistry C* **2010**, 114, (26), 11358-11363.
 100. Gemming, S.; Seifert, G.; Gotz, M.; Fischer, T.; Gantefor, G., Transition metal sulfide clusters below the cluster-platelet transition: Theory and experiment. *Physica Status Solidi B-Basic Solid State Physics* **2010**, 247, (5), 1069-1076.
 101. Gemming, S.; Enyashin, A. N.; Frenzel, J.; Seifert, G., Adsorption of nucleotides on the rutile (110) surface. *International Journal of Materials Research* **2010**, 101, (6), 758-764.
 102. Enyashin, A. N.; Seifert, G., Molecular-dynamics simulations of capillary imbibition of KI melt into MoS₂ nanotubes. *Chemical Physics Letters* **2010**, 501, (1-3), 98-102.
 103. Assfour, B.; Seifert, G., Hydrogen adsorption sites and energies in 2D and 3D covalent organic frameworks. *Chemical Physics Letters* **2010**, 489, (1-3), 86-91.
 104. Assfour, B.; Seifert, G., Adsorption of hydrogen in covalent organic frameworks: Comparison of simulations and experiments. *Microporous and Mesoporous Materials* **2010**, 133, (1-3), 59-65.
 105. Assfour, B.; Leoni, S.; Seifert, G., Hydrogen Adsorption Sites in Zeolite Imidazolate Frameworks ZIF-8 and ZIF-11. *Journal of Physical Chemistry C* **2010**, 114, (31), 13381-13384.
 106. Xiao, R.; Fritsch, D.; Kuzmin, M. D.; Koepernik, K.; Eschrig, H.; Richter, M.; Vietze, K.; Seifert, G., Co Dimers on Hexagonal Carbon Rings Proposed as Subnanometer Magnetic Storage Bits. *Physical Review Letters* **2009**, 103, (18), 187201.

107. Tenne, R.; Seifert, G., Recent Progress in the Study of Inorganic Nanotubes and Fullerene-Like Structures. *Annual Review of Materials Research* **2009**, 39, (1), 387-413.
108. Riedl, T.; Gemming, T.; Weissbach, T.; Seifert, G.; Gutmann, E.; Zschornak, M.; Meyer, D. C.; Gemming, S., ELNES study of chemical solution deposited SrO(SrTiO₃)(n) Ruddlesden-Popper films: Experiment and simulation. *Ultramicroscopy* **2009**, 110, (1), 26-32.
109. Rapacioli, M.; Spiegelman, F.; Talbi, D.; Mineva, T.; Goursot, A.; Heine, T.; Seifert, G., Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: Application to polycyclic aromatic hydrocarbon clusters. *The Journal of Chemical Physics* **2009**, 130, (24), 244304.
110. Oliveira, A. F.; Seifert, G.; Heine, T.; Duarte, H. A., Density-Functional Based Tight-Binding: an Approximate DFT Method. *Journal of the Brazilian Chemical Society* **2009**, 20, (7), 1193-1205.
111. Morawetz, K.; Gemming, S.; Luschtinetz, R.; Kunze, T.; Lipavsky, P.; Eng, L. M.; Seifert, G.; Pankoke, V.; Milde, P., Transport and noise in organic field-effect devices. *Physical Review B (Condensed Matter and Materials Physics)* **2009**, 79, (8), 085405.
112. Mitric, R.; Werner, U.; Wohlgemuth, M.; Seifert, G.; Bonacic-Koutecky, V., Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. *The Journal of Physical Chemistry A* **2009**, 113, (45), 12700-12705.
113. Luschtinetz, R.; Frenzel, J.; Milek, T.; Seifert, G., Adsorption of Phosphonic Acid at the TiO₂ Anatase (101) and Rutile (110) Surfaces. *The Journal of Physical Chemistry C* **2009**, 113, (14), 5730-5740.
114. Joswig, J.-O.; Seifert, G., Aspects of the Proton Transfer in Liquid Phosphonic Acid. *The Journal of Physical Chemistry B* **2009**, 113, (25), 8475-8480.
115. Gemming, S.; Seifert, G.; Bertram, N.; Fischer, T.; Goetz, M.; Gantefoer, G., One-dimensional (MoS₃)(n) clusters: Building blocks of clusters materials and ideal nanowires for molecular electronics. *Chemical Physics Letters* **2009**, 474, (1-3), 127-131.
116. Gemming, S.; Kunze, T.; Morawetz, K.; Pankoke, V.; Luschtinetz, R.; Seifert, G., The role of homophase and heterophase interfaces on transport properties in structured materials. *European Physical Journal-Special Topics* **2009**, 177, 83-101.
117. Frenzel, J.; Seifert, G.; Zahn, D., Surface Effects in the Pressure-Induced Structural Transformation of a ZnO Nanorod. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2009**, 635, (12), 1773-1776.
118. Enyashin, A. N.; Popov, I.; Seifert, G., Stability and electronic properties of Rhenium sulfide nanotubes. *physica status solidi (b)* **2009**, 246, (1), 114-118.
119. Enyashin, A. N.; Kreizman, R.; Seifert, G., Capillary Imbibition of PbI₂ Melt by Inorganic and Carbon Nanotubes. *The Journal of Physical Chemistry C* **2009**, 113, (31), 13664-13669.
120. Enyashin, A. N.; Bar-Sadan, M.; Sloan, J.; Houben, L.; Seifert, G., Nanoseashells and Nanooctahedra of MoS₂: Routes to Inorganic Fullerenes. *Chemistry of Materials* **2009**, 21, (23), 5627-5636.
121. Assfour, B.; Seifert, G., Hydrogen storage in 1D nanotube-like channels metal-organic frameworks: Effects of free volume and heat of adsorption on hydrogen uptake. *International Journal of Hydrogen Energy* **2009**, 34, (19), 8135-8143.
122. Zagorodniy, K.; Hermann, H.; Taut, M.; Seifert, G.; Zschech, E., Structure analysis and property improvements of the computer-simulated fullerene-based ultralow-k dielectrics. *Microelectronic Engineering* **2008**, 85, (10), 2118-2122.
123. Tenne, R.; Remskar, M.; Enyashin, A.; Seifert, G., Inorganic nanotubes and fullerene-like structures (IF). In *Topics in Applied Physics*, 2008; Vol. 111, pp 631-671.
124. Stefanov, M.; Enyashin, A. N.; Heine, T.; Seifert, G., Nanolubrication: How Do MoS₂-Based Nanostructures Lubricate? *Journal of Physical Chemistry C* **2008**, 112, (46), 17764-17767.

125. Seifert, G., Quantum molecular dynamics - The physics of explosive chemistry. *Nature Physics* **2008**, 4, (1), 12-13.
126. Popov, I.; Pecchia, A.; Okano, S.; Ranjan, N.; Di Carlo, A.; Seifert, G., Electronic and transport properties of contacts between molybdenum sulfide nanowires and gold electrodes. *Applied Physics Letters* **2008**, 93, (8), 083115.
127. Popov, I.; Gemming, S.; Okano, S.; Ranjan, N.; Seifert, G., Electromechanical Switch Based on Mo₆S₆ Nanowires. *Nano Letters* **2008**, 8, (12), 4093-4097.
128. Novak, P.; Chaplygin, I.; Seifert, G.; Gemming, S.; Laskowski, R., Ab-initio calculation of exchange interactions in YMnO₃. *Computational Materials Science* **2008**, 44, (1), 79-81.
129. Nagapriya, K. S.; Goldbart, O.; Kaplan-Ashiri, I.; Seifert, G.; Tenne, R.; Joselevich, E., Torsional Stick-Slip Behavior in WS₂ Nanotubes. *Physical Review Letters* **2008**, 101, (19), 195501.
130. Morawetz, K.; Gemming, S.; Luschtinetz, R.; Eng, L. M.; Seifert, G.; Kenfack, A., Current without external bias and diode effect in shuttling transport of nanoshafes. *New Journal of Physics* **2008**, 10, 103014.
131. Luschtinetz, R.; Oliveira, A. F.; Frenzel, J.; Joswig, J. O.; Seifert, G.; Duarte, H. A., Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. *Surface Science* **2008**, 602, (7), 1347-1359.
132. Kuc, A.; Heine, T.; Seifert, G.; Duarte, H. A., H₂ adsorption in metal-organic frameworks: Dispersion or electrostatic interactions? *Chemistry a European Journal* **2008**, 14, (22), 6597-6600.
133. Kuc, A.; Heine, T.; Seifert, G.; Duarte, H. A., On the nature of the interaction between H₂ and metal-organic frameworks. *Theoretical Chemistry Accounts* **2008**, 120, (4-6), 543-550.
134. Kibsgaard, J.; Tuxen, A.; Levisen, M.; Laegsgaard, E.; Gemming, S.; Seifert, G.; Lauritsen, J. V.; Besenbacher, F., Atomic-Scale Structure of Mo₆S₆ Nanowires. *Nano Letters* **2008**, 8, (11), 3928-3931.
135. Flecks, S.; Patallo, E. R.; Zhu, X. F.; Ernyei, A. J.; Seifert, G.; Schneider, A.; Dong, C. J.; Naismith, J. H.; van Pee, K. H., New Insights into the Mechanism of Enzymatic Chlorination of Tryptophan. *Angewandte Chemie-International Edition* **2008**, 47, (49), 9533-9536.
136. Deepak, F. L.; Popovitz-Biro, R.; Feldman, Y.; Cohen, H.; Enyashin, A.; Seifert, G.; Tenne, R., Fullerene-like Mo(W)_(1-x)Re_xS₂ nanoparticles. *Chemistry-an Asian Journal* **2008**, 3, (8-9), 1568-1574.
137. Bar Sadan, M.; Houben, L.; Wolf, S. G.; Enyashin, A.; Seifert, G.; Tenne, R.; Urban, K., Toward atomic-scale bright-field electron tomography for the study of fullerene-like nanostructures. *Nano Letters* **2008**, 8, (3), 891-896.
138. Bar Sadan, M.; Houben, L.; Enyashin, A. N.; Seifert, G.; Tenne, R., Atom by atom: HRTEM insights into inorganic nanotubes and fullerene-like structures. *Proceedings of the National Academy of Sciences of the United States of America* **2008**, 105, (41), 15643-15648.
139. Baburin, I. A.; Leoni, S.; Seifert, G., Enumeration of not-yet-synthesized zeolitic zinc imidazolate MOF networks: A topological and DFT approach. *Journal of Physical Chemistry B* **2008**, 112, (31), 9437-9443.
140. Zobelli, A.; Gloter, A.; Ewels, C. P.; Seifert, G.; Colliex, C., Electron knock-on cross section of carbon and boron nitride nanotubes. *Physical Review B* **2007**, 75, (24), 245402.
141. Zobelli, A.; Ewels, C. P.; Gloter, A.; Seifert, G., Vacancy migration in hexagonal boron nitride. *Physical Review B* **2007**, 75, (9), 094104.
142. Zahn, D.; Hochrein, O.; Kawska, A.; Seifert, G.; Grin, Y.; Kniep, R.; Leoni, S., Extending the scope of 'in silico experiments': Theoretical approaches for the investigation of reaction mechanisms, nucleation events and phase transitions. *Science and Technology of Advanced Materials* **2007**, 8, (5), 434-441.

143. Zagorodniy, K.; Hermann, H.; Taut, M.; Wang, Y.; Seifert, G.; Zschech, E., Structure and physical properties of computer-simulated fullerene-based ultralow k dielectric materials. *Stress-Induced Phenomena in Metallization* **2007**, 945, 162-169.
144. Seifert, G., Tight-binding density functional theory: An approximate Kohn-Sham DFT Scheme. *Journal of Physical Chemistry A* **2007**, 111, (26), 5609-5613.
145. Rapacioli, M.; Barthel, R.; Heine, T.; Seifert, G., Car-Parrinello treatment for an approximate density-functional theory method. *Journal of Chemical Physics* **2007**, 126, (12), 124103.
146. Popov, I.; Yang, T.; Berber, S.; Seifert, G.; Tomanek, D., Unique structural and transport properties of molybdenum chalcogenide nanowires. *Physical Review Letters* **2007**, 99, (8), 085503.
147. Popov, I.; Kunze, T.; Gemming, S.; Seifert, G., Self-assembly of Mo₆S₈ clusters on the Au(111) surface. *European Physical Journal D* **2007**, 45, (3), 439-446.
148. Popov, I.; Gemming, S.; Seifert, G., Structural and electronic properties of Mo₆S₈ clusters deposited on a Au(111) surface investigated with density functional theory. *Physical Review B* **2007**, 75, (24), 245436.
149. Milosevic, I.; Nikolic, B.; Dobardzic, E.; Damnjanovic, M.; Popov, I.; Seifert, G., Electronic properties and optical spectra of MoS₂ and WS₂ nanotubes. *Physical Review B* **2007**, 76, (23), 233414.
150. Mandumpal, J.; Gemming, S.; Seifert, G., Curvature effects of nitrogen on graphitic sheets: Structures and energetics. *Chemical Physics Letters* **2007**, 447, (1-3), 115-120.
151. Luschtinetz, R.; Seifert, G.; Jaehne, E.; Adler, H. J. P., Infrared spectra of alkylphosphonic acid bound to aluminium surfaces. *Macromolecular Symposia* **2007**, 254, 248-253.
152. Kuc, A.; Zhechkov, L.; Patchkovskii, S.; Seifert, G.; Heine, T., Hydrogen sieving and storage in fullerene intercalated graphite. *Nano Letters* **2007**, 7, (1), 1-5.
153. Kuc, A.; Enyashin, A.; Seifert, G., Metal-organic frameworks: Structural, energetic, electronic, and mechanical properties. *Journal of Physical Chemistry B* **2007**, 111, (28), 8179-8186.
154. Kohler, C.; Frauenheim, T.; Hourahine, B.; Seifert, G.; Sternberg, M., Treatment of collinear and noncollinear electron spin within an approximate density functional based method. *Journal of Physical Chemistry A* **2007**, 111, (26), 5622-5629.
155. Kaplan-Ashiri, I.; Cohen, S. R.; Apter, N.; Wang, Y. K.; Seifert, G.; Wagner, H. D.; Tenne, R., Microscopic investigation of shear in multiwalled nanotube deformation. *Journal of Physical Chemistry C* **2007**, 111, (24), 8432-8436.
156. Joswig, J. O.; Hazebroucq, S.; Seifert, G., Properties of the phosphonic-acid molecule and the proton transfer in the phosphonic-acid dimer. *Journal of Molecular Structure-Theochem* **2007**, 816, (1-3), 119-123.
157. Ivanovskaya, V. V.; Zobelli, A.; Seifert, G.; Ivanovskii, A. L., Dimensionally, morphologically, and thermally induced phase transformations in boron-nitrogen nanowires. *Jetp Letters* **2007**, 85, (12), 626-631.
158. Ivanovskaya, V. V.; Kohler, C.; Seifert, G., 3d metal nanowires and clusters inside carbon nanotubes: Structural, electronic, and magnetic properties. *Physical Review B* **2007**, 75, (7), 075410
159. Hentsche, M.; Hermann, H.; Lindackers, D.; Seifert, G., Microstructure and low-temperature hydrogen storage capacity of ball-milled graphite. *International Journal of Hydrogen Energy* **2007**, 32, (10-11), 1530-1536.
160. Guimaraes, L.; Enyashin, A. N.; Frenzel, J.; Heine, T.; Duarte, H. A.; Seifert, G., Imogolite nanotubes: Stability, electronic, and mechanical properties. *Acs Nano* **2007**, 1, (4), 362-368.
161. Gemming, S.; Seifert, G., Nanocrystals - Catalysts on the edge. *Nature Nanotechnology* **2007**, 2, (1), 21-22.

162. Gemming, S.; Luschtinetz, R.; Chaplygin, I.; Seifert, G.; Loppacher, C.; Eng, L. M.; Kunze, T.; Olbrich, C., Polymorphism in ferroic functional elements - Bridging length and time scales. *European Physical Journal-Special Topics* **2007**, *149*, 145-171.
163. Gemming, S.; Luschtinetz, R.; Alsheimer, W.; Seifert, G.; Loppacher, C.; Eng, L. M., Modelling ferroic functional elements. *Journal of Computer-Aided Materials Design* **2007**, *14*, 211-218.
164. Frenzel, J.; Joswig, J. O.; Seifert, G., Optical excitations in cadmium sulfide nanoparticles. *Journal of Physical Chemistry C* **2007**, *111*, (29), 10761-10770.
165. Enyashin, A. N.; Seifert, G., Titanium oxide fullerenes: electronic structure and basic trends in their stability. *Physical Chemistry Chemical Physics* **2007**, *9*, (43), 5772-5775.
166. Enyashin, A. N.; Gemming, S.; Seifert, G., DNA-wrapped carbon nanotubes. *Nanotechnology* **2007**, *18*, (24), 245702.
167. Enyashin, A. N.; Gemming, S.; Bar-Sadan, M.; Popovitz-Biro, R.; Hong, S. Y.; Prior, Y.; Tenne, R.; Seifert, G., Structure and stability of molybdenum sulfide fullerenes. *Angewandte Chemie-International Edition* **2007**, *46*, (4), 623-627.
168. Enyashin, A.; Gemming, S.; Seifert, G., Nanosized allotropes of molybdenum disulfide. *European Physical Journal-Special Topics* **2007**, *149*, 103-125.
169. Baldoni, M.; Leoni, S.; Sgamellotti, A.; Seifert, G.; Mercuri, F., Formation, structure, and polymorphism of novel lowest-dimensional AgI nanoaggregates by encapsulation in carbon nanotubes. *Small* **2007**, *3*, (10), 1730-1734.
170. Zobelli, A.; Ewels, C. P.; Gloter, A.; Seifert, G.; Stephan, O.; Csillag, S.; Colliex, C., Defective structure of BN nanotubes: From single vacancies to dislocation lines. *Nano Letters* **2006**, *6*, (9), 1955-1960.
171. Zhechkov, L.; Heine, T.; Seifert, G., Physisorption of N₂ on graphene platelets: An ab initio study. *International Journal of Quantum Chemistry* **2006**, *106*, (6), 1375-1382.
172. Wang, Y. K.; Seifert, G.; Hermann, H., Molecular design of fullerene-based ultralow-k dielectrics. *Physica Status Solidi a-Applications and Materials Science* **2006**, *203*, (15), 3868-3872.
173. Seifert, G.; Tamuliene, J.; Gemming, S., MonS_{2n+x} clusters-magic numbers and platelets. *Computational Materials Science* **2006**, *35*, (3), 316-320.
174. Seifert, G., Sr., Tight-binding density functional theory: An approximate Kohn-Sham DFT scheme. *Abstracts of Papers of the American Chemical Society* **2006**, *232*, 121-121.
175. Rother, A.; Reibold, M.; Lichte, H.; Leisegang, T.; Levin, A. A.; Paufler, P.; Meyer, D. C.; Gemming, S.; Chaplygin, I.; Seifert, G.; Ormeci, A.; Rosner, H., X-ray investigation, high-resolution electron holography, and density functional calculations of single-crystalline BaTiO₃. *Physical Review B* **2006**, *74*, (13), 134116.
176. Ranjan, N.; Seifert, G., Transport properties of functionalized carbon nanotubes: Density-functional Green's function calculations. *Physical Review B* **2006**, *73*, (15), 153408
177. Loppacher, C.; Zerweck, U.; Eng, L. M.; Gemming, S.; Seifert, G.; Olbrich, C.; Morawetz, K.; Schreiber, M., Adsorption of PTCDA on a partially KBr covered Ag(111) substrate. *Nanotechnology* **2006**, *17*, (6), 1568-1573.
178. Kuc, A.; Seifert, G., Hexagon-preserving carbon foams: Properties of hypothetical carbon allotropes. *Physical Review B* **2006**, *74*, (21), 214104.
179. Koskinen, P.; Hakkinen, H.; Seifert, G.; Sanna, S.; Frauenheim, T.; Moseler, M., Density-functional based tight-binding study of small gold clusters. *New Journal of Physics* **2006**, *8*, 9.
180. Kohler, C.; Seifert, G.; Frauenheim, T., Magnetism and the potential energy hypersurfaces of Fe-53 to Fe-57. *Computational Materials Science* **2006**, *35*, (3), 297-301.
181. Koeber, C.; Seifert, G.; Frauenheim, T., Spinpolarization in the SCC-DFTB formalism. *Abstracts of Papers of the American Chemical Society* **2006**, *232*, 130-130.
182. Kaplan-Ashiri, I.; Cohen, S. R.; Gartsman, K.; Ivanovskaya, V.; Heine, T.; Seifert, G.; Wiesel, I.; Wagner, H. D.; Tenne, R., On the mechanical behavior of WS₂ nanotubes under axial tension and

- compression. *Proceedings of the National Academy of Sciences of the United States of America* **2006**, 103, (3), 523-528.
183. Ivanovskaya, V. V.; Seifert, G.; Ivanovskii, A. L., Electronic structure of niobium-doped molybdenum disulfide nanotubes. *Russian Journal of Inorganic Chemistry* **2006**, 51, (2), 320-324.
184. Ivanovskaya, V. V.; Heine, T.; Gemming, S.; Seifert, G., Structure, stability and electronic properties of composite Mo_{1-x}Nb_xS₂ nanotubes. *Physica Status Solidi B-Basic Solid State Physics* **2006**, 243, (8), 1757-1764.
185. Goswami, B.; Pal, S.; Sarkar, P.; Seifert, G.; Springborg, M., Theoretical study of structural, electronic, and optical properties of ZnMnS_n clusters. *Physical Review B* **2006**, 73, (20), 205312.
186. Gemming, S.; Tamuliene, J.; Seifert, G.; Bertram, N.; Kim, Y. D.; Gantefor, G., Electronic and geometric structures of MoxSy and WxSy (x=1, 2, 4; y=1-12) clusters. *Applied Physics a-Materials Science & Processing* **2006**, 82, (1), 161-166.
187. Gemming, S.; Seifert, G.; Vilfan, I., Li doped Mo₆S₆ nanowires: elastic and electronic properties. *Physica Status Solidi B-Basic Solid State Physics* **2006**, 243, (13), 3320-3324.
188. Gemming, S.; Seifert, G., SrTiO₃(001)/vertical bar LaAlO₃(001) multilayers: A density-functional investigation. *Acta Materialia* **2006**, 54, (16), 4299-4306.
189. Gemming, S.; Seifert, G., Density-functional study of Mo₄S₆ on Au(111). *Applied Physics a-Materials Science & Processing* **2006**, 82, (1), 175-179.
190. Enyashin, A. N.; Seifert, G.; Ivanovskii, A. L., Simulation of the structural and thermal properties of tubular nanocrystallites of magnesium oxide. *Physics of the Solid State* **2006**, 48, (4), 801-805.
191. Enyashin, A. N.; Ivanovskii, A. L.; Seifert, G., Stability and electronic properties of single-walled gamma-AlO(OH) nanotubes. *Mendeleev Communications* **2006**, (6), 292-294.
192. Enyashin, A.; Gemming, S.; Heine, T.; Seifert, G.; Zhechkov, L., C-28 fullerenes - structure, electronic properties and intercalates. *Physical Chemistry Chemical Physics* **2006**, 8, (28), 3320-3325.
193. De Abreu, H. A.; De Almeida, W. B.; Duarte, H. A.; Fischer, G.; Heine, T.; Merino, G.; Seifert, G., Theoretical study of the propagation barrier of ethylene polymerization with TiR₂ (R = OCH₃ or CN): The importance of the beta-agostic interactions. *Journal of Molecular Structure-Theochem* **2006**, 762, (1-3), 9-15.
194. Bertram, N.; Cordes, J.; Kim, Y. D.; Gantefor, G.; Gemming, S.; Seifert, G., Nanoplatelets made from MoS₂ and WS₂. *Chemical Physics Letters* **2006**, 418, (1-3), 36-39.
195. Bar-Sadan, M.; Enyashin, A. N.; Gemming, S.; Popovitz-Biro, R.; Hong, S. Y.; Prior, Y.; Tenne, R.; Seifert, G., Structure and stability of molybdenum sulfide fullerenes. *Journal of Physical Chemistry B* **2006**, 110, (50), 25399-25410.
196. Zhechkov, L.; Heine, T.; Patchkovskii, S.; Seifert, G.; Duarte, H. A., An efficient a Posteriori treatment for dispersion interaction in density-functional-based tight binding. *Journal of Chemical Theory and Computation* **2005**, 1, (5), 841-847.
197. Tamuliene, J.; Seifert, G., Isomers of endohedral fullerene Sc-2@C-84. *Fullerenes Nanotubes and Carbon Nanostructures* **2005**, 13, (4), 279-286.
198. Seifert, G.; Enyashin, A. N.; Heine, T., Hyperdiamond and hyperlonsdaleit: Possible crystalline phases of fullerene C-28. *Physical Review B* **2005**, 72, (1), 012102
199. Sarkar, P.; Springborg, M.; Seifert, G., A theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core/shell nanoparticles. *Chemical Physics Letters* **2005**, 405, (1-3), 103-107.
200. Ruck, M.; Hoppe, D.; Wahl, B.; Simon, P.; Wang, Y. K.; Seifert, G., Fibrous red phosphorus. *Angewandte Chemie-International Edition* **2005**, 44, (46), 7616-7619.
201. Perez, N.; Heine, T.; Barthel, R.; Seifert, G.; Vela, A.; Mendez-Rojas, M. A.; Merino, G., Planar tetracoordinate carbons in cyclic hydrocarbons. *Organic Letters* **2005**, 7, (8), 1509-1512.

202. Patchkovskii, S.; Tse, J. S.; Yurchenko, S. N.; Zhechkov, L.; Heine, T.; Seifert, G., Graphene nanostructures as tunable storage media for molecular hydrogen. *Proceedings of the National Academy of Sciences of the United States of America* **2005**, 102, (30), 10439-10444.
203. Kohler, C.; Seifert, G.; Frauenheim, T., Density functional based calculations for Fe-n ($n \leq 32$). *Chemical Physics* **2005**, 309, (1), 23-31.
204. Kaplan-Ashiri, I.; Cohen, S. R.; Gartsman, K.; Rosentsveig, R.; Ivanovskaya, V.; Heine, T.; Seifert, G.; Wagner, H. D.; Tenne, R., Direct tensile tests of individual WS₂ nanotubes. In *Prism 5: The Fifth Pacific Rim International Conference on Advanced Materials and Processing, Pts 1-5*, Zhong, Z. Y., Ed. 2005; Vol. 475-479, pp 4097-4102.
205. Ivanovskaya, V. V.; Seifert, G.; Ivanovskii, A. L., Electronic structure of titanium disulfide nanostructures: Monolayers, nanostripes, and nanotubes. *Semiconductors* **2005**, 39, (9), 1058-1065.
206. Ivanovskaya, V. V.; Ranjan, N.; Heine, T.; Merino, G.; Seifert, G., Molecular dynamics study of the mechanical and electronic properties of carbon nanotubes. *Small* **2005**, 1, (4), 399-402.
207. Hermann, H.; Zagorodniy, K.; Touzick, A.; Taut, M.; Seifert, G., Computer simulation of fullerene-based ultra-low k dielectrics. *Microelectronic Engineering* **2005**, 82, (3-4), 387-392.
208. Heine, T.; Corminboeuf, C.; Seifert, G., The magnetic shielding function of molecules and π -electron delocalization. *Chemical Reviews* **2005**, 105, (10), 3889-3910.
209. Hazebroucq, S.; Picard, G. S.; Adamo, C.; Heine, T.; Gemming, S.; Seifert, G., Density-functional-based molecular-dynamics simulations of molten salts. *Journal of Chemical Physics* **2005**, 123, (13), 134510.
210. Gemming, S.; Seifert, G.; Muhle, C.; Jansen, M.; Albu-Yaron, A.; Arad, T.; Tenne, R., Electron microscopy, spectroscopy, and first-principles calculations Of Cs₂O. *Journal of Solid State Chemistry* **2005**, 178, (4), 1190-1196.
211. Gemming, S.; Lehmann, M.; Seifert, G., Semi-flexible star-shaped molecules: conformational analysis of nano-segregated mesogens forming columnar liquid-crystal phases. *Zeitschrift Fur Metallkunde* **2005**, 96, (9), 988-997.
212. Frenzel, J.; Oliveira, A. F.; Duarte, H. A.; Heine, T.; Seifert, G., Structural and electronic properties of bulk gibbsite and gibbsite surfaces. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2005**, 631, (6-7), 1267-1271.
213. Frenzel, J.; Joswig, J. O.; Sarkar, P.; Seifert, G.; Springborg, M., The effects of organisation, embedding and surfactants on the properties of cadmium chalcogenide (CdS, CdSe and CdS/CdSe) semiconductor nanoparticles. *European Journal of Inorganic Chemistry* **2005**, (18), 3585-3596.
214. Francke, M.; Hermann, H.; Wenzel, R.; Seifert, G.; Wetzig, K., Modification of carbon nanostructures by high energy ball-milling under argon and hydrogen atmosphere. *Carbon* **2005**, 43, (6), 1204-1212.
215. Fischer, G.; Barthel, R.; Seifert, G., Molecular dynamics study of the reaction $C_3+H_3(+)$. *European Physical Journal D* **2005**, 35, (3), 479-481.
216. Enyashin, A. N.; Seifert, G.; Ivanovskii, A. L., Electronic, structural, and thermal properties of a nanocable consisting of carbon and BN nanotubes. *Jetp Letters* **2005**, 80, (9), 608-611.
217. Enyashin, A. N.; Seifert, G.; Ivanovskii, A. L., Calculation of the electronic and thermal properties of C/BN nanotubular heterostructures. *Inorganic Materials* **2005**, 41, (6), 595-603.
218. Enyashin, A. N.; Seifert, G., Structure, stability and electronic properties of TiO₂ nanostructures. *Physica Status Solidi B-Basic Solid State Physics* **2005**, 242, (7), 1361-1370.
219. Duarte, H. A.; Heine, T.; Seifert, G., DFT x TB - a unified quantum-mechanical hybrid method. *Theoretical Chemistry Accounts* **2005**, 114, (1-3), 68-75.
220. Zhechkov, L.; Heine, T.; Seifert, G., D-5h C-50 fullerene: A building block for oligomers and solids? *Journal of Physical Chemistry A* **2004**, 108, (52), 11733-11739.

221. Zahn, D.; Seifert, G., Atomistic simulation study of the pressure induced incorporation of helium into C-60. *Journal of Physical Chemistry B* **2004**, 108, (42), 16495-16498.
222. Terentyev, A.; Scholz, R.; Schreiber, M.; Seifert, G., Theoretical investigation of excited states of C-3. *Journal of Chemical Physics* **2004**, 121, (12), 5767-5776.
223. Seifert, G., Hydrogen on and in carbon nanostructures. *Solid State Ionics* **2004**, 168, (3-4), 265-269.
224. Seifert, G., Nanomaterials - Nanocluster magic. *Nature Materials* **2004**, 3, (2), 77-78.
225. Merino, G.; Heine, T.; Seifert, G., The induced magnetic field in cyclic molecules. *Chemistry-a European Journal* **2004**, 10, (17), 4367-4371.
226. Krause, M.; Hulman, M.; Kuzmany, H.; Dubay, O.; Kresse, G.; Vietze, K.; Seifert, G.; Wang, C.; Shinohara, H., Fullerene quantum gyroscope. *Physical Review Letters* **2004**, 93, (13), 137403.
227. Kohler, T.; Frauenheim, T.; Hajnal, Z.; Seifert, G., Tubular structures of GaS. *Physical Review B* **2004**, 69, (19), 193403.
228. Kaplan-Ashiri, I.; Cohen, S. R.; Gartsman, K.; Rosentsveig, R.; Seifert, G.; Tenne, R., Mechanical behavior of individual WS₂ nanotubes. *Journal of Materials Research* **2004**, 19, (2), 454-459.
229. Ivanovskaya, V. V.; Seifert, G., Tubular structures of titanium disulfide TiS₂. *Solid State Communications* **2004**, 130, (3-4), 175-180.
230. Heine, T.; Zhechkov, L.; Seifert, G., Hydrogen storage by physisorption on nanostructured graphite platelets. *Physical Chemistry Chemical Physics* **2004**, 6, (5), 980-984.
231. Heine, T.; Vietze, K.; Seifert, G., C-13 NMR fingerprint characterizes long time-scale structure of Sc₃N@C₈₀ endohedral fullerene. *Magnetic Resonance in Chemistry* **2004**, 42, S199-S201.
232. Gemming, S.; Seifert, G.; Schreiber, M., Density-functional investigation of gold-coated metallic nanowires. *Physical Review B* **2004**, 69, (24), 245410.
233. Gemming, S.; Schreiber, M.; Thiel, W.; Heine, T.; Seifert, G.; de Abreu, H. A.; Duarte, H. A., Tunable discotic building blocks for liquid crystalline displays. *Journal of Luminescence* **2004**, 108, (1-4), 143-147.
234. Frenzel, J.; Gemming, S.; Seifert, G., Electronic structure of Ga-84 cluster compounds. *Physical Review B* **2004**, 70, (23), 235404.
235. Corminboeuf, C.; Heine, T.; Seifert, G.; Schleyer, P. V.; Weber, J., Induced magnetic fields in aromatic n -annulenes - interpretation of NICS tensor components. *Physical Chemistry Chemical Physics* **2004**, 6, (2), 273-276.
236. Bertram, N.; Kim, Y. D.; Gantefor, G.; Sun, Q.; Jena, P.; Tamuliene, J.; Seifert, G., Experimental and theoretical studies on inorganic magic clusters: M₄X₆ (M = W, Mo, X = O, S). *Chemical Physics Letters* **2004**, 396, (4-6), 341-345.
237. Ponomarenko, O.; Radny, M. W.; Smith, P. V.; Seifert, G., Properties of boron carbide nanotubes: Density-functional-based tight-binding calculations. *Physical Review B* **2003**, 67, (12), 125401.
238. Joswig, J. O.; Seifert, G.; Niehaus, T. A.; Springborg, M., Optical properties of cadmium sulfide clusters. *Journal of Physical Chemistry B* **2003**, 107, (13), 2897-2902.
239. Heine, T.; Schleyer, P. V.; Corminboeuf, C.; Seifert, G.; Reviakine, R.; Weber, J., Analysis of aromatic delocalization: Individual molecular orbital contributions to nucleus-independent chemical shifts. *Journal of Physical Chemistry A* **2003**, 107, (33), 6470-6475.
240. Hacoen, Y. R.; Popovitz-Biro, R.; Prior, Y.; Gemming, S.; Seifert, G.; Tenne, R., Synthesis of NiCl₂ nanotubes and fullerene-like structures by laser ablation: theoretical considerations and comparison with MoS₂ nanotubes. *Physical Chemistry Chemical Physics* **2003**, 5, (8), 1644-1651.
241. Grobert, N.; Seeger, T.; Seifert, G.; Ruhle, M., Processing, characterisation and theory of carbon nanotubes containing SiO_x-based nanocomposites. *Journal of Ceramic Processing Research* **2003**, 4, (1), 1-5.
242. Gemming, S.; Seifert, G., Nanotube bundles from calcium disilicide: A density functional theory study. *Physical Review B* **2003**, 68, (7), 075416

243. Chen, Z. F.; Jiao, H. J.; Seifert, G.; Horn, A. H. C.; Yu, D. K.; Clark, T.; Thiel, W.; Schleyer, P. V., The structure and stability of Si-60 and Ge-60 cages: A computational study. *Journal of Computational Chemistry* **2003**, 24, (8), 948-953.
244. Seifert, G.; Kohler, T.; Tenne, R., Stability of metal chalcogenide nanotubes. *Journal of Physical Chemistry B* **2002**, 106, (10), 2497-2501.
245. Seeger, T.; Kohler, T.; Frauenheim, T.; Grobert, N.; Terrones, M.; Seifert, G.; Ruhle, M., SiO₂-coated carbon nanotubes: theory and experiment. *Zeitschrift Fur Metallkunde* **2002**, 93, (5), 455-458.
246. Seeger, T.; Kohler, T.; Frauenheim, T.; Grobert, N.; Ruhle, M.; Terrones, M.; Seifert, G., Nanotube composites: novel SiO₂ coated carbon nanotubes. *Chemical Communications* **2002**, (1), 34-35.
247. Scheffer, L.; Rosentzveig, R.; Margolin, A.; Popovitz-Biro, R.; Seifert, G.; Cohen, S. R.; Tenne, R., Scanning tunneling microscopy study of WS₂ nanotubes. *Physical Chemistry Chemical Physics* **2002**, 4, (11), 2095-2098.
248. Frauenheim, T.; Seifert, G.; Elstner, M.; Niehaus, T.; Kohler, C.; Amkreutz, M.; Sternberg, M.; Hajnal, Z.; Di Carlo, A.; Suhai, S., Atomistic simulations of complex materials: ground-state and excited-state properties. *Journal of Physics-Condensed Matter* **2002**, 14, (11), 3015-3047.
249. Fabian, J.; Diaz, L. A.; Seifert, G.; Niehaus, T., Calculation of excitation energies of organic chromophores: a critical evaluation. *Journal of Molecular Structure-Theochem* **2002**, 594, 41-53.
250. Di Carlo, A.; Gheorghe, M.; Lugli, P.; Sternberg, M.; Seifert, G.; Frauenheim, T., Theoretical tools for transport in molecular nanostructures. *Physica B-Condensed Matter* **2002**, 314, (1-4), 86-90.
251. Bobadova-Parvanova, P.; Jackson, K. A.; Srinivas, S.; Horoi, M.; Kohler, C.; Seifert, G., Scanning the potential energy surface of iron clusters: A novel search strategy. *Journal of Chemical Physics* **2002**, 116, (9), 3576-3587.
252. Abdurahman, A.; Shukla, A.; Seifert, G., Ab initio many-body calculations of static dipole polarizabilities of linear carbon chains and chainlike boron clusters. *Physical Review B* **2002**, 66, (15), 155423.
253. Seifert, G.; Kohler, T.; Urbassek, H. M.; Hernandez, E.; Frauenheim, T., Tubular structures of silicon. *Physical Review B* **2001**, 63, (19), 193409.
254. Seifert, G.; Kohler, T.; Hajnal, Z.; Frauenheim, T., Tubular structures of germanium. *Solid State Communications* **2001**, 119, (12), 653-657.
255. Seifert, G.; Heine, T.; Fowler, P. W., Inorganic nanotubes and fullerenes - Structure and properties of hypothetical phosphorus fullerenes. *European Physical Journal D* **2001**, 16, (1-3), 341-343.
256. Seifert, G.; Frauenheim, T.; Kohler, T.; Urbassek, H. M., Tubular structures of siloxenes. *Physica Status Solidi B-Basic Research* **2001**, 225, (2), 393-399.
257. Rao, B. K.; Jena, P.; Burkart, S.; Gantefor, G.; Seifert, G., AlH₃ and Al₂H₆: Magic clusters with unmagical properties. *Physical Review Letters* **2001**, 86, (4), 692-695.
258. Niehaus, T. A.; Suhai, S.; Della Sala, F.; Lugli, P.; Elstner, M.; Seifert, G.; Frauenheim, T., Tight-binding approach to time-dependent density-functional response theory. *Physical Review B* **2001**, 63, (8), 085108.
259. Munch, W.; Kreuer, K. D.; Silvestri, W.; Maier, J.; Seifert, G., The diffusion mechanism of an excess proton in imidazole molecule chains: first results of an ab initio molecular dynamics study. *Solid State Ionics* **2001**, 145, (1-4), 437-443.
260. Lee, S. M.; An, K. H.; Lee, Y. H.; Seifert, G.; Frauenheim, T., A hydrogen storage mechanism in single-walled carbon nanotubes. *Journal of the American Chemical Society* **2001**, 123, (21), 5059-5063.
261. Lee, S. M.; An, K. H.; Lee, Y. H.; Seifert, G.; Frauenheim, T., Novel mechanism of hydrogen storage in carbon nanotubes. *Journal of the Korean Physical Society* **2001**, 38, (6), 686-691.

262. Lee, S. M.; An, K. H.; Kim, W. S.; Lee, Y. H.; Park, Y. S.; Seifert, G.; Frauenheim, T., Hydrogen storage in carbon nanotubes. *Synthetic Metals* **2001**, 121, (1-3), 1189-1190.
263. Krause, M.; Kuzmany, H.; Georgi, P.; Dunsch, L.; Vietze, K.; Seifert, G., Structure and stability of endohedral fullerene Sc₃N@C-80: A Raman, infrared, and theoretical analysis. *Journal of Chemical Physics* **2001**, 115, (14), 6596-6605.
264. Kohler, C.; Seifert, G.; Gerstmann, U.; Elstner, M.; Overhof, H.; Frauenheim, T., Approximate density-functional calculations of spin densities in large molecular systems and complex solids. *Physical Chemistry Chemical Physics* **2001**, 3, (23), 5109-5114.
265. Joswig, J. O.; Springborg, M.; Seifert, G., Structural and electronic properties of small titanium-carbon clusters (metcars). *Physical Chemistry Chemical Physics* **2001**, 3, (23), 5130-5134.
266. Hermann, H.; Fugaciu, F.; Seifert, G., Towards controlled production of specific carbon nanostructures - a theoretical study on structural transformations of graphitic and diamond particles. *Applied Physics Letters* **2001**, 79, (1), 63-65.
267. Heine, T.; Zerbetto, F.; Seifert, G.; Fowler, P. W., Isomers of C-70 dimer. *Journal of Physical Chemistry A* **2001**, 105, (7), 1140-1143.
268. Heine, T.; Goursoot, A.; Seifert, G.; Webert, J., Performance of DFT for Si-29 NMR chemical shifts of silanes. *Journal of Physical Chemistry A* **2001**, 105, (3), 620-626.
269. Amkreutz, M.; Jungnickel, G.; Seifert, G.; Kohler, T.; Frauenheim, T., On the structural and electronic properties of fluorinated carbon allotropes. *New Diamond and Frontier Carbon Technology* **2001**, 11, (3), 207-220.
270. Alippi, P.; Colombo, L.; Ruggerone, P.; Sieck, A.; Seifert, G.; Frauenheim, T., Atomic-scale characterization of boron diffusion in silicon. *Physical Review B* **2001**, 64, (7), 075207
271. Seifert, G.; Terrones, H.; Terrones, M.; Jungnickel, G.; Frauenheim, T., On the electronic structure of WS(2) nanotubes. *Solid State Communications* **2000**, 114, (5), 245-248.
272. Seifert, G.; Terrones, H.; Terrones, M.; Jungnickel, G.; Frauenheim, T., Structure and electronic properties of MoS(2) nanotubes. *Physical Review Letters* **2000**, 85, (1), 146-149.
273. Seifert, G.; Terrones, H.; Terrones, M.; Frauenheim, T., Novel NbS(2) metallic nanotubes. *Solid State Communications* **2000**, 115, (12), 635-638.
274. Seifert, G.; Kohler, T.; Frauenheim, T., Molecular wires, solenoids, and capacitors by sidewall functionalization of carbon nanotubes. *Applied Physics Letters* **2000**, 77, (9), 1313-1315.
275. Seifert, G.; Hernandez, E., Theoretical prediction of phosphorus nanotubes. *Chemical Physics Letters* **2000**, 318, (4-5), 355-360.
276. Seifert, G.; Frauenheim, T., On the stability of non carbon nanotubes. *Journal of the Korean Physical Society* **2000**, 37, (2), 89-92.
277. Rogers, K. M.; Fowler, P. W.; Seifert, G., Chemical versus steric frustration in boron nitride heterofullerene polyhedra. *Chemical Physics Letters* **2000**, 332, (1-2), 43-50.
278. Munch, W.; Kreuer, K. D.; Seifert, G.; Maier, J., Proton diffusion in perovskites: comparison between BaCeO₃, BaZrO₃, SrTiO₃, and CaTiO₃ using quantum molecular dynamics. *Solid State Ionics* **2000**, 136, 183-189.
279. Joswig, J. O.; Springborg, M.; Seifert, G., Structural and electronic properties of cadmium sulfide clusters. *Journal of Physical Chemistry B* **2000**, 104, (12), 2617-2622.
280. Heine, T.; Zerbetto, F.; Seifert, G.; Fowler, P. W., C-13 NMR patterns of odd-numbered C-119 fullerenes. *Journal of Physical Chemistry A* **2000**, 104, (17), 3865-3868.
281. Heine, T.; Buhl, M.; Fowler, P. W.; Seifert, G., Modelling the C-13 NMR chemical shifts of C-84 fullerenes. *Chemical Physics Letters* **2000**, 316, (5-6), 373-380.
282. Haugk, M.; Elsner, J.; Frauenheim, T.; Staab, T. E. M.; Latham, C. D.; Jones, R.; Leipner, H. S.; Heine, T.; Seifert, G.; Sternberg, M., Structures, energetics and electronic properties of complex III-V semiconductor systems. *Physica Status Solidi B-Basic Research* **2000**, 217, (1), 473-511.

283. Frauenheim, T.; Seifert, G.; Elstner, M.; Hajnal, Z.; Jungnickel, G.; Porezag, D.; Suhai, S.; Scholz, R., A self-consistent charge density-functional based tight-binding method for predictive materials simulations in physics, chemistry and biology. *Physica Status Solidi B-Basic Research* **2000**, *217*, (1), 41-62.
284. Elstner, M.; Frauenheim, T.; Kaxiras, E.; Seifert, G.; Suhai, S., A self-consistent charge density-functional based tight-binding scheme for large biomolecules. *Physica Status Solidi B-Basic Research* **2000**, *217*, (1), 357-376.
285. Boltalina, O. V.; Ioffe, I. N.; Sidorov, L. N.; Seifert, G.; Vietze, K., Ionization energy of fullerenes. *Journal of the American Chemical Society* **2000**, *122*, (40), 9745-9749.
286. Munch, W.; Kreuer, K. D.; Seifert, G.; Majer, J., A quantum molecular dynamics study of proton diffusion in SrTiO₃ and CaTiO₃. *Solid State Ionics* **1999**, *125*, (1-4), 39-45.
287. Munch, W.; Kreuer, K. D.; Adams, S.; Seifert, G.; Maier, J., The relation between crystal structure and the formation and mobility of protonic charge carriers in perovskite-type oxides: A case study of Y-doped BaCeO₃ and SrCeO₃. *Phase Transitions* **1999**, *68*, (3), 567-586.
288. Heine, T.; Seifert, G.; Fowler, P. W.; Zerbetto, F., A tight-binding treatment for C-13 NMR spectra of fullerenes. *Journal of Physical Chemistry A* **1999**, *103*, (43), 8738-8746.
289. Heine, T.; Fowler, P. W.; Seifert, G., C-36: from dimer to bulk. *Solid State Communications* **1999**, *111*, (1), 19-22.
290. Heine, T.; Fowler, P. W.; Rogers, K. M.; Seifert, G., Structural and energetic parallels between hydrogenated and fluorinated fullerenes: C₃₆H₆. *Journal of the Chemical Society-Perkin Transactions 2* **1999**, (4), 707-711.
291. Haugk, M.; Elsner, J.; Heine, T.; Frauenheim, T.; Seifert, G., A parallel code for a self-consistent charge density functional based tight binding method: Total energy calculations for extended systems. *Computational Materials Science* **1999**, *13*, (4), 239-251.
292. Fugaciu, F.; Hermann, H.; Seifert, G., Concentric-shell fullerenes and diamond particles: A molecular-dynamics study. *Physical Review B* **1999**, *60*, (15), 10711-10714.
293. Fowler, P. W.; Rogers, K. M.; Seifert, G.; Terrones, M.; Terrones, H., Pentagonal rings and nitrogen excess in fullerene-based BN cages and nanotube caps. *Chemical Physics Letters* **1999**, *299*, (5), 359-367.
294. Fowler, P. W.; Heine, T.; Rogers, K. M.; Sandall, J. P. B.; Seifert, G.; Zerbetto, F., C-36, a hexavalent building block for fullerene compounds and solids. *Chemical Physics Letters* **1999**, *300*, (3-4), 369-378.
295. Burkart, S.; Blessing, N.; Klipp, B.; Muller, J.; Gantefor, G.; Seifert, G., Experimental verification of the high stability of Al₁₃H: a building block of a new type of cluster material? *Chemical Physics Letters* **1999**, *301*, (5-6), 546-550.
296. Albertazzi, E.; Domene, C.; Fowler, P. W.; Heine, T.; Seifert, G.; Van Alsenoy, C.; Zerbetto, F., Pentagon adjacency as a determinant of fullerene stability. *Physical Chemistry Chemical Physics* **1999**, *1*, (12), 2913-2918.
297. Seifert, G.; Kaschner, R.; Schone, M.; Pastore, G., Density functional calculations for Zintl systems: structure, electronic structure and electrical conductivity of liquid NaSn alloys. *Journal of Physics-Condensed Matter* **1998**, *10*, (6), 1175-1198.
298. Seifert, G.; Bartl, A.; Dunsch, L.; Ayuela, A.; Rockenbauer, A., Electron spin resonance spectra: geometrical and electronic structure of endohedral fullerenes. *Applied Physics a-Materials Science & Processing* **1998**, *66*, (3), 265-271.
299. Krause, M.; Dunsch, L.; Seifert, G.; Fowler, P. W.; Gromov, A.; Kratschmer, W.; Gutierrez, R.; Porezag, D.; Frauenheim, T., Vibrational signatures of fullerene oxides. *Journal of the Chemical Society-Faraday Transactions* **1998**, *94*, (16), 2287-2294.

300. Kietzmann, H.; Rochow, R.; Gantefor, G.; Eberhardt, W.; Vietze, K.; Seifert, G.; Fowler, P. W., Electronic structure of small fullerenes: Evidence for the high stability of C-32. *Physical Review Letters* **1998**, 81, (24), 5378-5381.
301. Kaschner, R.; Becker, J. S.; Seifert, G., Theoretical and mass spectrometric investigations of the formation of calcium fluoride cluster ions. *International Journal of Mass Spectrometry* **1998**, 176, (1-2), 103-111.
302. Elstner, M.; Porezag, D.; Jungnickel, G.; Elsner, J.; Haugk, M.; Frauenheim, T.; Suhai, S.; Seifert, G., Self-consistent-charge density-functional tight-binding method for simulations of complex materials properties. *Physical Review B* **1998**, 58, (11), 7260-7268.
303. Seifert, G.; Fowler, P. W.; Mitchell, D.; Porezag, D.; Frauenheim, T., Boron-nitrogen analogues of the fullerenes: Electronic and structural properties. *Chemical Physics Letters* **1997**, 268, (5-6), 352-358.
304. Porezag, D.; Jungnickel, G.; Frauenheim, T.; Seifert, G.; Ayuela, A.; Pederson, M. R., Theoretical investigations of homo- and heteronuclear bridged fullerene oligomers. *Applied Physics a-Materials Science & Processing* **1997**, 64, (3), 321-326.
305. Munch, W.; Seifert, G.; Kreuer, K. D.; Maier, J., A quantum molecular dynamics study of the cubic phase of BaTiO₃ and BaZrO₃. *Solid State Ionics* **1997**, 97, (1-4), 39-44.
306. Kaschner, R.; Frauenheim, T.; Köhler, T.; Seifert, G., A density-functional-based tight-binding scheme for the study of silicon-oxygen compounds. *Journal of Computer-Aided Materials Design* **1997**, 4, 53-62.
307. Jones, R. O.; Seifert, G., Structure and bonding in carbon clusters C-14 to C-24: Chains, rings, bowls, plates, and cages. *Physical Review Letters* **1997**, 79, (3), 443-446.
308. Fowler, P. W.; Mitchell, D.; Taylor, R.; Seifert, G., Structures and energetics of dimeric fullerene and fullerene oxide derivatives. *Journal of the Chemical Society-Perkin Transactions 2* **1997**, (10), 1901-1905.
309. Fowler, P. W.; Mitchell, D.; Seifert, G.; Zerbetto, F., Energetics of fullerenes with octagonal rings. *Fullerene Science and Technology* **1997**, 5, (4), 747-768.
310. Domene, M. C.; Fowler, P. W.; Mitchell, D.; Seifert, G.; Zerbetto, F., Energetics of C-20 and C-22 fullerene and near-fullerene carbon cages. *Journal of Physical Chemistry A* **1997**, 101, (44), 8339-8344.
311. Bartl, A.; Dunsch, L.; Kirbach, U.; Seifert, G., Paramagnetic states of metals and C-13 in isolated endohedral fullerenes. *Synthetic Metals* **1997**, 86, (1-3), 2395-2396.
312. Ayuela, A.; Seifert, G.; Schmidt, R., Electronic structure of Lanthanum-carbon clusters. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters* **1997**, 41, (1), 69-72.
313. Widany, J.; Frauenheim, T.; Kohler, T.; Stemberg, M.; Porezag, D.; Jungnickel, G.; Seifert, G., Density-functional-based construction of transferable nonorthogonal tight-binding potentials for B, N, BN, BH, and NH. *Physical Review B* **1996**, 53, (8), 4443-4452.
314. Seifert, G.; Vietze, K.; Schmidt, R., Ionization energies of fullerenes - Size and charge dependence. *Journal of Physics B-Atomic Molecular and Optical Physics* **1996**, 29, (21), 5183-5192.
315. Seifert, G.; Porezag, D.; Frauenheim, T., Calculations of molecules, clusters, and solids with a simplified LCAO-DFT-LDA scheme. *International Journal of Quantum Chemistry* **1996**, 58, (2), 185-192.
316. Seifert, G.; Gutierrez, R.; Schmidt, R., Ionization energies and Coulomb explosion of highly charged C-60. *Physics Letters A* **1996**, 211, (6), 357-362.
317. Rohmund, F.; Campbell, E. E. B.; Knospe, O.; Seifert, G.; Schmidt, R., Collision energy dependence of molecular fusion and fragmentation in C-60(+)+C-60 collisions. *Physical Review Letters* **1996**, 76, (18), 3289-3292.
318. Munch, W.; Seifert, G.; Kreuer, K. D.; Maier, J., A quantum molecular dynamics study of proton conduction phenomena in BaCeO₃. *Solid State Ionics* **1996**, 86-8, 647-652.

319. Knospe, O.; Glotov, A. V.; Seifert, G.; Schmidt, R., Theoretical studies of atomic cluster-cluster collisions. *Journal of Physics B-Atomic Molecular and Optical Physics* **1996**, 29, (21), 5163-5174.
320. Kaschner, R.; Schone, M.; Seifert, G.; Pastore, G., Ab initio simulations of liquid systems: Concentration dependence of the electric conductivity of NaSn alloys. *Journal of Physics-Condensed Matter* **1996**, 8, (43), L653-L657.
321. Gutierrez, R.; Frauenheim, T.; Kohler, T.; Seifert, G., Stability of silicon carbide structures: From clusters to solid surfaces. *Journal of Materials Chemistry* **1996**, 6, (10), 1657-1663.
322. Gausa, M.; Kaschner, R.; Seifert, G.; Faehrmann, J. H.; Lutz, H. O.; MeiwesBroer, K. H., Photoelectron investigations and density functional calculations of anionic Sb-n(-) and Bi-n(-) clusters. *Journal of Chemical Physics* **1996**, 104, (24), 9719-9728.
323. Fowler, P. W.; Heine, T.; Mitchell, D.; Schmidt, R.; Seifert, G., Boron-nitrogen analogues of the fullerenes: The isolated-square rule. *Journal of the Chemical Society-Faraday Transactions* **1996**, 92, (12), 2197-2201.
324. Fowler, P. W.; Heine, T.; Mitchell, D.; Orlandi, G.; Schmidt, R.; Seifert, G.; Zerbetto, F., Energetics of fullerenes with heptagonal rings. *Journal of the Chemical Society-Faraday Transactions* **1996**, 92, (12), 2203-2210.
325. Fowler, P. W.; Heine, T.; Manolopoulos, D. E.; Mitchell, D.; Orlandi, G.; Schmidt, R.; Seifert, G.; Zerbetto, F., Energetics of fullerenes with four-membered rings. *Journal of Physical Chemistry* **1996**, 100, (17), 6984-6991.
326. Becker, J. S.; Seifert, G.; Saprykin, A. I.; Dietze, H. J., Mass spectrometric and theoretical investigations into the formation of argon molecular ions in plasma mass spectrometry. *Journal of Analytical Atomic Spectrometry* **1996**, 11, (9), 643-648.
327. Ayuela, A.; Fowler, P. W.; Mitchell, D.; Schmidt, R.; Seifert, G.; Zerbetto, F., C-62: Theoretical evidence for a nonclassical fullerene with a heptagonal ring. *Journal of Physical Chemistry* **1996**, 100, (39), 15634-15636.
328. Schulte, J.; Knospe, O.; Seifert, G.; Schmidt, R., C-60(+)+C-60 COLLISIONS .2. MASS AND ANGULAR-DISTRIBUTIONS. *Physics Letters A* **1995**, 198, (1), 51-54.
329. Schone, M.; Kaschner, R.; Seifert, G., AB-INITIO SIMULATIONS OF LIQUID NASN ALLOYS - ZINTL ANIONS AND NETWORK FORMATION. *Journal of Physics-Condensed Matter* **1995**, 7, (3), L19-L26.
330. Porezag, D.; Frauenheim, T.; Kohler, T.; Seifert, G.; Kaschner, R., CONSTRUCTION OF TIGHT-BINDING-LIKE POTENTIALS ON THE BASIS OF DENSITY-FUNCTIONAL THEORY - APPLICATION TO CARBON. *Physical Review B* **1995**, 51, (19), 12947-12957.
331. Kaschner, R.; Saalman, U.; Seifert, G.; Gausa, M., DENSITY-FUNCTIONAL CALCULATIONS OF STRUCTURES AND IONIZATION ENERGIES FOR HEAVY GROUP-V CLUSTER ANIONS. *International Journal of Quantum Chemistry* **1995**, 56, (6), 771-777.
332. Frauenheim, T.; Weich, F.; Kohler, T.; Uhlmann, S.; Porezag, D.; Seifert, G., DENSITY-FUNCTIONAL-BASED CONSTRUCTION OF TRANSFERABLE NONORTHOGONAL TIGHT-BINDING POTENTIALS FOR SI AND SIH. *Physical Review B* **1995**, 52, (15), 11492-11501.
333. Seifert, G.; Schulte, J., ON THE FORMATION OF DEUTERIUM FULLERENE COMPLEXES IN COLLISIONS OF C-60 WITH D-2. *Physics Letters A* **1994**, 188, (4-6), 365-370.
334. Schulte, J.; Seifert, G., DFT-LDA MOLECULAR-DYNAMICS OF MOLECULAR COLLISION PROCESSES. *Chemical Physics Letters* **1994**, 221, (3-4), 230-236.
335. Schmidt, R.; Schulte, J.; Knospe, O.; Seifert, G., C+60+C60 COLLISIONS .1. MULTIFRAGMENTATION AND COLLECTIVE FLOW EFFECTS. *Physics Letters A* **1994**, 194, (1-2), 101-105.
336. Kaschner, R.; Seifert, G., INVESTIGATIONS OF HYDROGEN-BONDED SYSTEMS - LOCAL-DENSITY APPROXIMATION AND GRADIENT CORRECTIONS. *International Journal of Quantum Chemistry* **1994**, 52, (4), 957-961.

337. Gausa, M.; Kaschner, R.; Lutz, H. O.; Seifert, G.; Meiwesbroer, K. H., PHOTOELECTRON AND THEORETICAL INVESTIGATIONS ON BISMUTH AND ANTIMONY PENTAMER ANIONS - EVIDENCE FOR AROMATIC STRUCTURE. *Chemical Physics Letters* **1994**, 230, (1-2), 99-102.
338. Seifert, G.; Jones, R. O., STRUCTURE OF PHOSPHORUS CLUSTERS BY SIMULATED ANNEALING. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters* **1993**, 26, (1-4), 349-351.
339. Seifert, G.; Schmidt, R., MOLECULAR-DYNAMICS AND TRAJECTORY CALCULATIONS - THE APPLICATION OF AN LCAO-LDA SCHEME FOR SIMULATIONS OF CLUSTER-CLUSTER COLLISIONS. *New Journal of Chemistry* **1992**, 16, (12), 1145-1147.
340. Seifert, G.; Schmidt, R., FUSION AND DEEP INELASTIC-SCATTERING IN C-60-C-60 COLLISIONS. *International Journal of Modern Physics B* **1992**, 6, (23-24), 3845-3851.
341. Seifert, G.; Pastore, G.; Car, R., ABINITIO MOLECULAR-DYNAMICS SIMULATION OF LIQUID NASN ALLOY. *Journal of Physics-Condensed Matter* **1992**, 4, (11), L179-L183.
342. Seifert, G.; Jones, R. O., CAGE MOLECULES CONTAINING ELEMENTS OF GROUP-V AND GROUP-VI .2. MOLECULAR-DYNAMICS STUDY OF P4S3 AND P-7(3-). *Journal of Chemical Physics* **1992**, 96, (4), 2951-2952.
343. Jones, R. O.; Seifert, G., CAGE MOLECULES CONTAINING ELEMENTS OF GROUP-V AND GROUP-VI .1. STRUCTURE DETERMINATIONS USING SIMULATED ANNEALING. *Journal of Chemical Physics* **1992**, 96, (4), 2942-2950.
344. Jones, R. O.; Seifert, G., STRUCTURE OF PHOSPHORUS CLUSTERS USING SIMULATED ANNEALING .2. P9, P10, P11, ANIONS P4(2-), P10(2-), P11(3-), AND CATIONS PN(+) TO N = 11. *Journal of Chemical Physics* **1992**, 96, (10), 7564-7572.
345. Blaudeck, P.; Frauenheim, T.; Porezag, D.; Seifert, G.; Fromm, E., A METHOD AND RESULTS FOR REALISTIC MOLECULAR DYNAMIC SIMULATION OF HYDROGENATED AMORPHOUS-CARBON STRUCTURES USING A SCHEME CONSISTING OF A LINEAR COMBINATION OF ATOMIC ORBITALS WITH THE LOCAL-DENSITY APPROXIMATION. *Journal of Physics-Condensed Matter* **1992**, 4, (30), 6389-6400.
346. Seifert, G.; Schmidt, R.; Lutz, H. O., CLUSTER CLUSTER COLLISIONS .2. CLUSTER MOLECULES - A STABLE STATE OF MATTER. *Physics Letters A* **1991**, 158, (5), 237-241.
347. Seifert, G.; Jones, R. O., GEOMETRIC AND ELECTRONIC-STRUCTURE OF CLUSTERS. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters* **1991**, 20, (1-4), 77-80.
348. Schmidt, R.; Seifert, G.; Lutz, H. O., CLUSTER CLUSTER COLLISIONS .1. REACTION CHANNELS - FUSION, DEEP INELASTIC AND QUASI-ELASTIC COLLISIONS. *Physics Letters A* **1991**, 158, (5), 231-236.
349. Hietschold, M.; Seifert, G.; Hamann, C., SHAPE OF THE LEAD-PHTHALOCYANINE (PB-PC) MOLECULE AND THE FIELD-INDUCED SWITCHING EFFECT IN MONOCLINIC PB-PC. *Synthetic Metals* **1991**, 42, (3), 2625-2628.
350. Friedrich, K.; Seifert, G.; Grossmann, G., NUCLEAR MAGNETIC SHIELDING IN MOLECULES - THE APPLICATION OF GIAOS IN LCAO-X-ALPHA-CALCULATIONS. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters* **1990**, 17, (1), 45-46.
351. Eschrig, H.; Seifert, G., CORRELATED ELECTRONIC-STRUCTURE OF THE HIGH-TC SUPERCONDUCTOR RE1BA2CU3O7-X PHASE AND POSSIBLE INTERLAYER PAIRING. *Physica Scripta* **1989**, T25, 88-90.
352. Seifert, G.; Schwab, B.; Becker, S.; Dietze, H. J., ON THE FORMATION OF BORON NITROGEN CLUSTERS IN A LASER-INDUCED PLASMA. *International Journal of Mass Spectrometry and Ion Processes* **1988**, 85, (3), 327-338.
353. Seifert, G.; Becker, S.; Dietze, H. J., CARBON CLUSTER IONS IN LASER-INDUCED PLASMA. *International Journal of Mass Spectrometry and Ion Processes* **1988**, 84, (1-2), 121-133.
354. Knospe, O.; Schmidt, R.; Seifert, G., PERCOLATION APPROACH FOR ATOMIC AND MOLECULAR CLUSTER FORMATION. *Physics Letters A* **1988**, 129, (4), 236-240.

355. Friedrich, K.; Grossmann, G.; Seifert, G., APPROXIMATE VARIANT FOR THE CALCULATION OF THE NUCLEAR MAGNETIC SCREENING OF MOLECULES BY THE UCP-X-ALPHA-METHOD. *Zeitschrift Fur Chemie* **1988**, 28, (4), 156-157.
356. Eschrig, H.; Seifert, G., ELECTRONIC-STRUCTURE ANALYSIS OF LNBA₂CU₃O₇-X - IMPLICATIONS ON NORMAL CONDUCTIVITY AND SUPERCONDUCTIVITY. *Solid State Communications* **1988**, 65, (12), 1525-1527.
357. Eschrig, H.; Seifert, G., ELECTRONIC-STRUCTURE ANALYSIS OF LNBA₂CU₃O₇-X - IMPLICATIONS ON NORMAL AND SUPERCONDUCTIVITY. *Physica C* **1988**, 153, 1243-1244.
358. Seifert, G., ON THE ELECTRONIC SHELL STRUCTURE OF COPPER CLUSTERS. *Physica Status Solidi B-Basic Research* **1987**, 143, (1), K37-K42.
359. Fritsche, H. G.; Seifert, G.; Muller, H., CARBON ON AND IN PALLADIUM - CLUSTER ORBITAL STUDIES ON X-ALPHA POTENTIAL CALCULATIONS. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1987**, 268, (1), 65-80.
360. Eschrig, H.; Seifert, G., ELECTRONIC-STRUCTURE CALCULATIONS FOR OXOCUPRATE CLUSTERS OF THE HIGH-TC SUPERCONDUCTING PHASES. *Solid State Communications* **1987**, 64, (4), 521-525.
361. Seifert, G.; Eschrig, H.; Bieger, W., AN APPROXIMATION VARIANT OF LCAO-X-ALPHA METHODS. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1986**, 267, (3), 529-539.
362. Seifert, G., ELECTRONIC-STRUCTURE AND MAGIC NUMBER OF ALKALINE METAL-CLUSTERS. *Zeitschrift Fur Physik D-Atoms Molecules and Clusters* **1986**, 4, (2), 207-208.
363. Seifert, G.; Eschrig, H., LCAO-X-ALPHA CALCULATIONS OF TRANSITION-METAL CLUSTERS. *Physica Status Solidi B-Basic Research* **1985**, 127, (2), 573-585.
364. Hietschold, V.; Seifert, G., SOFT-X-RAY SPECTRA OF AMORPHOUS HYDROGENATED SILICON. *Physica Status Solidi B-Basic Research* **1985**, 129, (2), K163-K166.
365. Eschrig, H.; Seifert, G.; Ziesche, P., CURRENT-DENSITY FUNCTIONAL THEORY OF QUANTUM ELECTRODYNAMICS. *Solid State Communications* **1985**, 56, (9), 777-780.
366. Bieger, W.; Seifert, G.; Eschrig, H.; Grossmann, G., CALCULATION OF THE ELEMENTARY STATE PROPERTIES OF SMALL MOLECULES BY MEANS OF AN LCAO-XALPHA PROCEDURE. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1985**, 266, (4), 751-763.
367. Bieger, W.; Seifert, G.; Eschrig, H.; Grossmann, G., LCAO X-ALPHA CALCULATIONS OF NUCLEAR MAGNETIC SHIELDING IN MOLECULES. *Chemical Physics Letters* **1985**, 115, (3), 275-280.
368. Seifert, G.; Fritsche, H. G.; Ziesche, P.; Heera, V., ON THE ELECTRONIC-STRUCTURE OF PALLADIUM HYDROGEN AND PLATINUM HYDROGEN SYSTEMS. *Physica Status Solidi B-Basic Research* **1984**, 121, (2), 705-715.
369. Heera, V.; Seifert, G.; Ziesche, P., A SEMI-RELATIVISTIC VARIANT OF THE SCATTERED-WAVE X-ALPHA METHOD. *Journal of Physics B-Atomic Molecular and Optical Physics* **1984**, 17, (4), 519-530.
370. Bieger, W.; Grossmann, G.; Seifert, G., LCAO-X-ALPHA CALCULATIONS ON SMALL MOLECULES. *Zeitschrift Fur Chemie* **1984**, 24, (4), 156-157.
371. Heera, V.; Seifert, G.; Ziesche, P., SEMIRELATIVISTIC SCF-SW-X-ALPHA CALCULATIONS OF URANIUM-COMPOUNDS - ELECTRONIC-STRUCTURE AND CHEMICAL-BOND. *Physica Status Solidi B-Basic Research* **1983**, 118, (2), K107-K112.
372. Heera, V.; Seifert, G.; Ziesche, P., SEMIRELATIVISTIC SCF-SW-X-ALPHA CALCULATIONS OF URANIUM-COMPOUNDS - CHARGE-DENSITY DIFFERENCES AT THE URANIUM NUCLEUS. *Physica Status Solidi B-Basic Research* **1983**, 119, (1), K1-K4.
373. Muller, H.; Opitz, C.; Seifert, G., COMPARISON OF EHT AND SW-X-ALPHA CALCULATIONS. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1982**, 263, (5), 1005-1015.
374. Muller, H.; Opitz, C.; Seifert, G., COMPARISON OF EXTENDED HUCKEL THEORY CALCULATIONS AND SW-X-ALPHA CALCULATIONS - ELECTRON-STRUCTURE OF 3D-METAL ATOM, 4D-METAL

- ATOM AND 5D-METAL ATOM CLUSTERS. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1981**, 262, (6), 1073-1088.
375. Drager, G.; Brummer, O.; Heera, V.; Seifert, G.; Ziesche, P., POLARIZED TIK-BETA VALENCE BAND SPECTRA OF TIO₂ (RUTILE). *Physica Status Solidi B-Basic Research* **1981**, 104, (1), 219-226.
376. Thomas, B.; Seifert, G.; Grossmann, G., NMR SPECTROSCOPIC STUDIES ON N-15 LABELED HEXASUBSTITUTED CYCLOTRIPHOSPHAZATRIENES. *Zeitschrift Fur Chemie* **1980**, 20, (6), 217-217.
377. Seifert, G.; Grossmann, G.; Muller, H., SCF-SW-XALPHA-CALCULATIONS ON MOLYBDENUM-HALOGEN CLUSTER COMPOUNDS. *Journal of Molecular Structure* **1980**, 64, (MAY), 93-102.
378. Seifert, G.; Finster, J.; Muller, H., SW X-ALPHA CALCULATIONS AND X-RAY PHOTOELECTRON-SPECTRA OF MOLYBDENUM(II) CHLORIDE CLUSTER COMPOUNDS. *Chemical Physics Letters* **1980**, 75, (2), 373-377.
379. Hartmann, E.; Seifert, G., AN ASSESSMENT OF THE SCATTERED-WAVE CLUSTER TECHNIQUE BY CONSIDERING THE INTERNAL-CONVERSION OF TC-99M IN THE METAL. *Physica Status Solidi B-Basic Research* **1980**, 100, (2), 589-594.
380. Thomas, B.; Seifert, G.; Grossmann, G.; Scheller, D., NMR-SPECTROSCOPY OF N-15 LABELED CHLOROCYCLOPHOSPHAZENES. *Zeitschrift Fur Physikalische Chemie-Leipzig* **1979**, 260, (2), 225-235.
381. Muller, C.; Seifert, G.; Lautenschlager, G.; Wonn, H.; Ziesche, P.; Mrosan, E., BAND-STRUCTURE AND CLUSTER CALCULATIONS OF FEAL SYSTEMS. *Physica Status Solidi B-Basic Research* **1979**, 91, (2), 605-613.
382. Seifert, G.; Mrosan, E.; Muller, H.; Ziesche, P., SW-X-ALPHA CALCULATIONS OF SMALL NIOBIUM CLUSTERS. *Physica Status Solidi B-Basic Research* **1978**, 89, (2), K175-K178.
383. Seifert, G.; Mrosan, E.; Muller, H., ELECTRONIC-STRUCTURE OF 4D AND 5D TRANSITION-METAL CLUSTERS. *Physica Status Solidi B-Basic Research* **1978**, 89, (2), 553-560.
384. Seifert, G.; Grossmann, G., SCF-SW-X-ALPHA CALCULATION FOR P₄ MOLECULE. *Zeitschrift Fur Chemie* **1978**, 18, (6), 233-234.
385. Grossmann, G.; Gruner, M.; Seifert, G., O-NMR SPECTROSCOPIC STUDIES ON PHOSPHORYL COMPOUNDS .1. OPCL₃, OPCL₂X, OPCLX₂, OPX₃, X=F, BR, OCH₃, N(CH₃)₂. *Zeitschrift Fur Chemie* **1976**, 16, (9), 362-363.