

## Research Area C ‘Molecular Nanostructures’

### Project C1 ‘Synthesis and Structural Characterization of Molecule-Based Nanostructures’

#### C1.1 ,Synthesis and Structural Characterization of Molecule-Based Nanostructures‘ (D. Fenske, A. Eichhöfer, O. Fuhr)

- [C1.1:1] \* P. Sevillano, O. Fuhr, M. Kattanek, P. Nava, O. Hampe, S. Lebedkin, R. Ahlrichs, D. Fenske, and M. Kappes, *Die phosphoranstabilisierten Gold-Arsen-Cluster  $[Au_{19}(AsnPr)_8(dppe)_6]Cl_3$ ,  $[Au_{10}(AsnPr)_4(dppe)_4]Cl_2$ ,  $[Au_{17}(AsnPr)_6(As_2nPr_2)(dppm)_6]Cl_3$  und  $[Au_{10}(AsPh)_4(dppe)_4]Cl_2$  – Synthese, Charakterisierung und DFT-Rechnungen*, Angew. Chem. **118**, 3785–3791 (2006); Angew. Chem. Int. Ed. **45**, 3702 (2006)
- [C1.1:2] S. Chitsaz, D. Fenske, and O. Fuhr, *Silberchalkogenidcluster mit Dimethylanilinmercapto-Liganden: Synthesen und Kristallstrukturen von  $[Ag_{65}S_{13}(SC_6H_4NMe_2)_{39}(dppm)_5]$ ,  $[Ag_{76}Se_{13}(SC_6H_4NMe_2)_{50}(PPh_3)_{6.5}]$  und  $[Ag_{88}Se_{12}(SC_6H_4NMe_2)_{63}(PPh_3)_6]$* , Angew. Chem. **118**, 8224–8228 (2006); Angew. Chemie. Int. Ed. **45**, 8055 (2006)
- [C1.1:3] O. Fuhr, L. Fernandez-Recio, and D. Fenske, *A simple synthetic route to the formation of tetracopper(I) 2-mercaptopthiazoline compounds – The crystal structures of  $[Cu_4(S-thiaz)_4(PEt_2Ph)_2]$ ,  $[Cu_4(S-thiaz)_4PEt_3)_2$ ,  $[Cu_4(S-thiaz)_4]_4$ , and  $[Cu_4(S-thiaz)_4]_4$* , Can. J. Chem. **84**, 251 (2006)
- [C1.1:4] \* R. Ahlrichs, N.R.M. Crawford, A. Eichhöfer, D. Fenske, O. Hampe, M. Kappes, and J. Olkowska-Oetzel, *Synthesis and Structure of Two Ionic Copper Indium Selenolate Cluster Complexes  $[As(C_6H_5)_4]_2[Cu_6In_4(SeC_6H_5)_{16}Cl_4]$  and  $[As(C_6H_5)_4][Cu_7In_4(SeC_6H_5)_{20}]$* , Eur. J. Inorg. Chem. 345 (2006)
- [C1.1:5] \* R. Ahlrichs, D. Fenske, A. Rothenberger, C. Schrotte, and S. Wieber, *Atom Assignment in Solid-State Structures on the Basis of X-ray Crystallography and DFT Calculations – A Case Study on a Molecular Cu-Sb Alloy*, Eur. J. Inorg. Chem. 1127 (2006)
- [C1.1:6] ‡ Q.-F. Zhang, Z. Yu, J. Ding, Y. Song, A. Rothenberger, D. Fenske, and W.-H. Leung, *Construction of New Heteroselenometallic Clusters: Formation of Crownlike  $[Et_4N]_4(\mu_5-WSe_4)(CuI)_5(\mu-I)_2$  and Octahedral Polymeric  $[(\mu_6-WSe_4)Cu_5I_4(py)_4]_n$  from Planar  $[Et_4N]_4[(\mu_4-WSe_4)Cu_4I_6]$  with Additional Faces*, Inorg. Chem. **45**, 5187 (2006)
- [C1.1:7] ‡ D.A. Bashirov, O. Fuhr, and S.N. Konchenko, *Synthesis and Structure of new Heteronuclear Clusters  $[PPh_4][Fe_4Rh_3Se_2(CO)_{16}]$  and  $[PPh_4]_2[Fe_3Rh_4Te_2(CO)_{15}]$* , Russ. Chem. Bull., Int. Ed. **55**, 802 (2006)
- [C1.1:8] P. Sevillano, O. Fuhr, E. Matern, and D. Fenske, *Synthese, Kristallstruktur und spektroskopische Charakterisierung von  $[Au_{12}(PPh)_2(P_2Ph_2)_2(dppm)_4Cl_2]Cl_2$* , Z. Anorg. Allg. Chem. **632**, 735 (2006)
- [C1.1:9] M. Shafeai-Fallah, W. Shi, D. Fenske, and A. Rothenberger, *Synthesen und Kristallstrukturen von Übergangsmetallkomplexen mit Dithiophosphinato- und Trithiophosphonator-Liganden*, Z. Anorg. Allg. Chem. **632**, 1091 (2006)
- [C1.1:10] \* R. Ahlrichs, A. Eichhöfer, D. Fenske, K. May, and H. Sommer, *Molekülstruktur und theoretische Untersuchungen von  $(PPh_4)_2[Bi_{10}Cu_{10}(SPh)_{24}]$* , Angew. Chem. **119**, 8402 (2007); Angew. Chem. Int. Ed. **46**, 8254 (2007)
- [C1.1:11] D. Fenske, A. Rothenberger, and S. Wieber, *Synthesis and Characterization of the First Silver Complexes with Antimony Anions*, Eur. J. Inorg. Chem. 648 (2007)

- [C1.1:12] ‡ A. Eichhofer, P.T Wood, R. Viswanath, and R.A. Mole, *Synthesis, structure and magnetic behaviour of Manganese(II) selenolate complexes*  $[\text{Mn}(\text{SePh})_2]$ ,  $[\text{Mn}(\text{SePh})_2(\text{bipy})_2]$  and  $[\text{Mn}(\text{SePh})_2(\text{phen})_2]$  (*bipy* = bipyridyl, *phen* = phenanthroline), *Eur. J. Inorg. Chem.* **4794** (2007)
- [C1.1:13] \* P. Sevillano, O. Fuhr, O. Hampe, S. Lebedkin, C. Neiss, R. Ahlrichs, D. Fenske, and M.M. Kappes, *Synthesis, characterization and quantum mechanical calculations of*  $[\text{Au}_{18}\text{Se}_8(\text{dppthph})_6]\text{Cl}_2$ , *Eur. J. Inorg. Chem.* **5163** (2007)
- [C1.1:14] \* P. Sevillano, O. Fuhr, O. Hampe, S. Lebedkin, E. Matern, D. Fenske, and M.M. Kappes, *Synthesis, Characterization and X-Ray Structure Determination of*  $[\text{Au}_{18}(\text{P})_2(\text{PPh})_4(\text{PHPh})(\text{dppm})_6]\text{Cl}_3$ , *Inorg. Chem.* **46**, 7294 (2007)
- [C1.1:15] D. Fenske, I. Issac, and A. Rothenberger, *Towards Syntheses and Structures of Heterometallic Clusters Containing Tantalum-tetrachalcogenato Building Blocks*, *J. Cluster Science* **18**, 19 (2007)
- [C1.1:16] ‡ C. Nitschke, A.I. Wallbank, D. Fenske, and J.F. Corrigan, *Facile Synthesis of High Nuclearity Silver-Ferrocenyldiselenolate Clusters*, *J. Cluster Science* **18**, 131 (2007)
- [C1.1:17] ‡ D. Cave, J.F. Corrigan, A. Eichhöfer, D. Fenske, C.M. Kowalchuk, H. Rösner and P. Scheer, *Investigation of the Thermal Properties of a Series of Copper Selenide Cluster Molecules*, *J. Cluster Science* **18**, 157 (2007)
- [C1.1:18] ‡ O. Fuhr, L. Fernandez-Rezio, A. Castiñeras, and D. Fenske, *Synthese und Struktur der Cluster*  $[\text{Cu}_{50}\text{Se}_{24}(\text{S-thiaz})_2(\text{dppm})_{10}]$  und  $[\text{Cu}_{48}\text{Se}_{24})\text{S-thiazH}]_2(\text{dppm})_{10}$ , *Z. Anorg. Allg. Chem.* **633**, 700 (2007)
- [C1.1:19] \* S. König, A. Eichhöfer, N. Crawford, R. Ahlrichs, and D. Fenske, *Synthese, Kristallstruktur und quantenchemische Untersuchung des phosphanstabilisierten Nickel-Schwefel-Clusters*  $[\text{Ni}_{32}\text{S}_{24}(\text{PPh}_3)_{10}]$ , *Z. Anorg. Allg. Chem.* **633**, 713 (2007)
- [C1.1:20] P. Sevillano, O. Fuhr, and D. Fenske, *Synthese und Struktur von*  $[\text{Au}_{10}\text{Se}_5(\text{dppa})_4\{\text{Co}_2(\text{CO})_5\}_4]$ , *Z. Anorg. Allg. Chem.* **633**, 1783 (2007)
- [C1.1:21] B. Bechlars, R. Feuerhake, and D. Fenske, *Synthesen und Kristallstrukturen neuer chalcogenido-verbrückter Niob-Kupfer-Cluster*, *Z. Anorg. Allg. Chem.* **633**, 2603 (2007)
- [C1.1:22] \* C. Anson, A. Eichhöfer, I. Issac, D. Fenske, O. Fuhr, P. Sevillano, C. Persau, D. Stalke, and J. Zhang, *Synthesis and crystal structures of the ligand-stabilized silver chalcogenide clusters*  $[\text{Ag}_{154}\text{Se}_{77}(\text{dppxy})_{18}]$ ,  $[\text{Ag}_{320}(\text{StBu})_{60}\text{S}_{130}(\text{dppp})_{12}]$ ,  $[\text{Ag}_{352}\text{S}_{128}(\text{StC}_5\text{H}_{11})_{96}]$ , and  $[\text{Ag}_{490}\text{S}_{188}(\text{StC}_5\text{H}_{11})_{114}]$ , *Angew. Chem.* **120**, 1346 (2008); *Angew. Chem. Int. Ed.* **47**, 1326 (2008)
- [C1.1:23] ‡ A. Eichhöfer, P.T. Wood, R.N. Viswanath, and R.A. Mole, *Synthesis, structure and physical properties of the manganese(II) selenide/selenolate cluster complexes*  $[\text{Mn}_{32}\text{Se}_{14}(\text{SePh})_{36}(\text{PnPr}_3)_4]$  and  $[\text{Na}(\text{benzene-15-crown-5})(\text{C}_4\text{H}_8\text{O})_2]_2[\text{Mn}_8\text{Se}(\text{SePh})_{16}]$ , *Chem. Commun.* 1596 (2008)
- [C1.1:24] ‡ B. Bechlars, I. Issac, R. Feuerhake, R. Clérac, O. Fuhr, and D. Fenske, *Syntheses, Structures and Magnetic Properties of New Chalcogen-Bridged Heterodimetallic Clusters Compounds with Heterocubane Structure*, *Eur. J. Inorg. Chem.* 1632 (2008)
- [C1.1:25] C.T. Mitkina, N. Zakharchuk, D. Naumov, O. Gerasko, D. Fenske, and V. Fedin, *Syntheses, Structures, and Electrochemical Properties of Inclusion Compounds of Cucurbit[8]uril with Cobalt(III) and Nickel(II) Complexes*, *Inorg. Chem.* **47**, 6748 (2008)

- [C1.1:26] H. Sommer, A. Eichhöfer, and D. Fenske, *Synthese und Kristallstrukturen der Bismutchalkogenolate  $Bi(SC_6H_5)_3$ ,  $Bi(SeC_6H_5)_3$  und  $Bi(S-4-CH_3C_6H_4)_3$* , Z. Anorg. Allg. Chem. **634**, 436 (2008)
- [C1.1:27] \*‡ O.A. Gerasko, E.A. Maichineva, M.I. Naumova, M. Neumaier, M.M. Kappes, S. Lebedkin, D. Fenske, and V.P. Fedin, *Sandwich-Type Tetranuclear Lanthanide Complexes with Cucurbit[6]uril: From Molecular Compounds to Coordination Polymers*, Inorg. Chem. **47**, 8869 (2008)
- [C1.1:28] \* H. Sommer, A. Eichhöfer, N. Drebov, R. Ahlrichs, and D. Fenske, *Preparation, Geometric and Electronic Structures of  $[Bi_2Cu_4(SPh)_8(PPh_3)_4]$  with a  $Bi_2$  Dumbbell,  $[Bi_4Ag_3(SePh)_6Cl_3(PPh_3)_3]_2$  and  $[Bi_4Ag_3(SePh)_6X_3(PPhiPr_2)_3]_2$  ( $X=Cl, Br$ ) with a  $Bi_4$  Unit*, Eur. J. Inorg. Chem. 5138 (2008)
- [C1.1:29] L. Fernandez-Recio, D. Fenske, and O. Fuhr, *Copper Chalcogenide Cluster Compounds with Nitro-functionalized Ligand Shell*, Z. Anorg. Allg. Chem. **634**, 2853 (2008)
- [C1.1:30] H. Sommer, A. Eichhöfer, and D. Fenske, *Synthese und Kristallstrukturen der Bismutchalkogenolate  $Bi(SC_6H_5)_3$ ,  $Bi(SeC_6H_5)_3$  und  $Bi(S-4-CH_3C_6H_4)_3$* , Z. Anorg. Allg. Chem. **634**, 436 (2008)
- [C1.1:31] ‡ N.V. Izarova, M.N. Sokolov, D.G. Samsonenko, A. Rothenberger, D. Fenske, and V.P. Fedin, *Synthesis and Structures of two new coordination polymers formed by large polyoxometalate fragments and lanthanide cations*, Russian Chemical Bulletin **57**, 78 (2008)
- [C1.1:32] \*‡ D. Coucouvanis, A.R. Patal, Q. Zhang, N. Lehnert, R. Ahlrichs, K. Fink, D. Fenske, A.K. Powell, and Y. Lan, *Synthesis Electronic Structure, and Structural Characterization of the New, Non - Innocent 4.5- Dithio - Catecholate Ligand, its Metal Complexes, and Their Oxidized 4, 5- Dithio-o-quinone Derivatives*, Inorg. Chem. **48**, 8830 (2009)
- [C1.1:33] \* A. Eichhöfer, J. Olkowska-Oetzel, D. Fenske, K. Fink, V. Mereacre, A.K. Powell, and G. Butth, *Synthesis and Structure of an “Iron-Doped” Copper Selenide Cluster Molecule:  $[Cu_{30}Fe_2Se_6(SePh)_{24}(dppm)_4]$* , Inorg. Chem. **48**, 8977 (2009)
- [C1.1:34] ‡ C.-F. Zhuang, J. Zhang, Q. Wang, Z.-H. Chu, D. Fenske, and C.-Y. Su, *Temperature-Dependent Guest-Driven Single-Crystal-to-Single-Crystal Ligand Exchange in a Two-Fold Interpenetrated  $Cd^{II}$  Grid Network*, Chem. Eur. J. **15**, 7578 (2009)
- [C1.1:35] ‡ J.F. Corrigan, O. Fuhr, and D. Fenske, *Metal Chalcogenide Clusters on the Border between Molecules and Materials*, Adv. Mater. **21**, 1867 (2009)
- [C1.1:36] R. Langer, L. Wünsche, D. Fenske, and O. Fuhr, *Kupferchalkogenid-Clusterverbindungen mit Brom-funktionalisierter Ligandenhülle*, Z. Anorg. Allg. Chem. **635**, 2488 (2009)
- [C1.1:37] S. König, D. Fenske, and F. Weigend, *Synthesis, Crystal Structure and Bond Situation of  $[Co_7Se_7Cp_3(CO)_4]$  Cp = Cyclopentadienyl*, Z. Anorg. Allg. Chem. **635**, 2288 (2009)
- [C1.1:38] H. Sommer, A. Eichhöfer, and D. Fenske, *Synthesis, Crystal Structure and Thermal Behavior of  $[BiAg_3Br_6(PPh_3)_6]$  and  $[Bi_3Ag_6(SPh)_6Cl_3(PPhiPr_2)_3]$* , Z. Anorg. Allg. Chem. **635**, 1997 (2009)
- [C1.1:39] \* H. Sommer, N. Drebov, A. Eichhöfer, R. Ahlrichs, and D. Fenske, *Synthesis, Structures and Theoretical Investigations of  $[Li(thf)_4]_2$   $[Ti_2Cu_8S_4(SPh)_{10}]$  and  $[Ti_2Ag_6S_6Cl_2(PPhiPr_2)_6]$* , Eur. J. Inorg. Chem. 4329 (2009)

- [C1.1:40] ‡ M.-L. Fu, D. Fenske, B. Weinert, and O. Fuhr, *One-Dimensional Coordination Polymers Containing Polynuclear (Selenolato) copper Complexes Linked By Bipyridine Ligands*, Eur. J. Inorg. Chem. 1098 (2010)
- [C1.1:41] G. Schmid and D. Fenske, *Metal Clusters and Nanoparticles*, Phil. Trans. R. Soc. A **368**, 1207 (2010)
- [C1.1:42] ‡ A. Eichhöfer, J.-J. Jiang, H. Sommer, F. Weigend, O. Fuhr, D. Fenske, C.-Y. Su, and G. Buth, *1-D-Tin(II) Phenylchalcogenolato Complexes  $^1\text{A}[\text{Sn}(E\text{Ph})_2]$  ( $E = \text{S}, \text{Se}, \text{Te}$ ) – Synthesis, Structures, Quantum Chemical Studies and Thermal Behaviour*, Eur. J. Inorg. Chem. 410 (2010)
- [C1.1:43] ‡ J.-J. Jiang, L. Li, M.-H. Lan, M. Pan, A. Eichhöfer, D. Fenske, and C.-Y. Su, *Thermally Stable Porous Hydrogen-Bonded Coordination Networks Displaying Dual Properties Of Robustness and Dynamics Upon Guest Uptake*, Chem. Eur. J. **16**, 1841 (2010)
- [C1.1:44] \* ‡ C.B. Khadka, D.G. Macdonald, Y. Lan, A.K. Powell, D. Fenske, and J.F. Corrigan, *Trimethylsilylchalcogenolates of Co(II) and Mn(II); From Mononuclear Coordination Complexes to Cluster Containing  $-\text{ESiMe}_3$  Moieties ( $E = \text{S}, \text{Se}$ )*, Inorg. Chem. **49**, 7289 (2010)
- [C1.1:45] ‡ M.L. Fu, I. Issac, D. Fenske, and O. Fuhr, *Metal-Rich Copper Chalcogenide Clusters at the Border Between Molecule and Bulk Phase: The Structures of  $[\text{Cu}_{93}\text{Se}_{42}(\text{SeC}_6\text{H}_4\text{SMe})_9(\text{PPh}_3)_{18}]$ ,  $[\text{Cu}_{96}\text{Se}_{45}(\text{SeC}_6\text{H}_4\text{SMe})_6(\text{PPh}_3)_{18}]$ , and  $[\text{Cu}_{136}\text{S}_{56}(\text{SCH}_2\text{C}_4\text{H}_3\text{O})_{24}(\text{dpppt})_{10}]$* , Angew. Chem. Int. Ed. **49**, 6899 (2010)
- [C1.1:46] ‡ S. Dehnen, A. Eichhöfer, J. F. Corrigan, O. Fuhr, and D. Fenske, *Synthesis and Characterization of I-VI Nanoclusters, in Nanoparticles; From Theory to Application*; Ed. By G. Schmid, page 127-213, Wiley-VCH, Weinheim 2010
- [C1.1:47] ‡ M.-L. Fu, D. Fenske, B. Weinert, and O. Fuhr, *One-Dimensional Coordination Polymers Containing Polynuclear (Selenolato)copper Complexes Linked by Bipyridine Ligands*, Eur. J. Inorg. Chem. 1098 (2010)
- [C1.1:48] R. Langer, B. Breiting, O. Fuhr, L. Wünsche, and D. Fenske, *Functionalized Silver Cluster*, Z. Anorg. Allg. Chem. **637**, 995 (2011)
- [C1.1:49] ‡ X. Wang, J. Huang, S. Xiang, Y. Liu, J. Zhang, A. Eichhöfer, D. Fenske, S. Bai and C.-Y. Su, *Discrete  $\text{Ag}_6\text{L}_6$  coordination nanotubular structures based on a T-shaped pyridyl diphosphine*, Chem. Commun. **47**, 3849 (2011)
- [C1.1:50] R. Langer, W. Yu, L. Wünsche, G. Buth, O. Fuhr, and D. Fenske, *Synthese und Strukturaufklärung Trimethylsiloxy-funktionalisierter Kupferchalkogenidcluster*, Z. Anorg. Allg. Chem. **637**, 1834 (2011)
- [C1.1:51] ‡ S. Ahmar, C. Nitschke, N. Vijayaratnam, D.G. MacDonald, D. Fenske, and J.F. Corrigan, *A ferrocenylmethylselenolate complex of Ag(I): preparation of the polyferrocenyl cluster  $[\text{Ag}_8(\text{SeCH}_2\text{Fc})_8(\text{PPh}_3)_4]$  from the new silylated reagent  $\text{FcCH}_2\text{SeSiMe}_3$* , New J. Chem. **35**, 2013 (2011)

#### C1.4 ‘Nanoscale Hollow Spheres’ (C. Feldmann)

- [C1.4:1] \* C. Zimmerman, C. Feldmann, M. Wanner, and D. Gerthsen, *Nanoscale Gold Hollow Spheres via Microemulsion Approach*, *Small* **3**, 1347 (2007)
- [C1.4:2] D.H.M. Buchold and C. Feldmann, *Nanoscale AlO(OH) Hollow Spheres - Synthesis and Container-type Functionality*, *Nano Lett.* **7**, 3489 (2007)
- [C1.4:3] D.H.M. Buchold and C. Feldmann, *Microemulsion Approach to Non-agglomerated and Crystalline Nanomaterials*, *Adv. Funct. Mater.* **18**, 1002 (2008)
- [C1.4:4] D.H.M. Buchold and C. Feldmann, *Nanoscale Complex Metal Cyanides and Thermolysis thereof*, *Solid State Sci.* **10**, 1305 (2008)
- [C1.4:5] H. Gröger, F. Gyger, P. Leidinger, C. Zurmühl, and C. Feldmann, *Microemulsion Approach to Nanocontainers and its Variability in Composition and Filling*, *Adv. Mater.* **21**, 1586 (2009)
- [C1.4:6] H. Goesmann and C. Feldmann, *Nanoparticulate Functional Materials (Review)*, *Angew. Chem. Int. Ed.* **49**, 1362 (2010)
- [C1.4:7] F. Gyger, M. Hübner, C. Feldmann, N. Barsan, and U. Weimar, *Nanoscale SnO<sub>2</sub> Hollow Spheres and Their Application as a Gas-Sensing Material*, *Chem. Mater.* **22**, 4821 (2010)
- [C1.4:8] \* C. Kind, R. Popescu, E. Müller, D. Gerthsen, and C. Feldmann, *Microemulsion-based Synthesis of nanoscaled Silver Hollow Spheres and Direct Comparison to Massive Particles of Similar Size*, *Nanoscale* **2**, 2223 (2010)
- [C1.4:9] \* P. Leidinger, R. Popescu, D. Gerthsen, and C. Feldmann, *Nanoscale La(OH)<sub>3</sub> Hollow Spheres and Fine-tuning of Its Outer Diameter and Cavity Size*, *Small* **6**, 1886 (2010)
- [C1.4:10] H. Gröger, C. Kind, P. Leidinger, M. Roming, and C. Feldmann, *Nanoscale Hollow Spheres: Microemulsion-based Synthesis, Structural Characterization and Container-type Functionalities (Review)*, *Materials* **3**, 4355 (2010)
- [C1.4:11] \* C. Zurmühl, R. Popescu, D. Gerthsen, and C. Feldmann, *Microemulsion-based Synthesis of Nanoscale TiO<sub>2</sub> Hollow Spheres*, *Solid State Sci.* **13**, 1505 (2011)
- [C1.4:12] \* P. Leidinger, R. Popescu, D. Gerthsen, and C. Feldmann, *Nanoscale Copper Sulfide Hollow Spheres with precisely adjusted Phase Composition: Covellite (CuS), Digenite (Cu<sub>1.8</sub>S), Chalcocite (Cu<sub>2</sub>S)*, *Nanoscale* **3**, 2544 (2011)
- [C1.4:13] \* S. Indris, M. Scheuermann, S. Becker, V. Šepelák, R. Kruk, J. Suffner, F. Gyger, C. Feldmann, A.S. Ulrich, and H. Hahn, *Local Structural Disorder and Relaxation in SnO<sub>2</sub> Nanostructures Studied by <sup>119</sup>Sn MAS NMR and <sup>119</sup>Sn Mössbauer Spectroscopy*, *J. Phys. Chem. C* **115**, 6433 (2011)
- [C1.4:14] \* S. Simonato, H. Gröger, J. Möllmer, R. Staudt, A. Puls, F. Dreisbach, and C. Feldmann, *Reversible Sorption and Storage of CO<sub>2</sub> with Nanoscale γ-Al(OH) Hollow Spheres*, *Chem. Commun.* **48**, 844 (2012)

### C1.5 ,Oxo / Hyroxo Clusters of the Lanthanides for Potential Photonic and Magnetic Applications' (P. Roesky)

- [C1.5:1] \* ‡ M.T. Gamer, P.W. Roesky, S.N. Konchenko, P. Nava, and R. Ahlrichs, *Report on an Al-Eu and an Al-Yb Donor-Acceptor Bond*, Angew. Chem. **118**, 4558 (2006); Angew. Chem. Int. Ed. **45**, 4447 (2006)
- [C1.5:2] \* ‡ M. Wiecko, P.W. Roesky, P. Nava, R. Ahlrichs, and S.N. Konchenko, *Gallium(I)-Alkaline Earth Metal Donor-Acceptor bonds*, Chem. Commun. 927 (2007)
- [C1.5:3] \* ‡ M.T. Gamer, Y. Lan, P.W. Roesky, A.K. Powell, and R. Clérac, *A Pentanuclear Dysprosium Hydroxy Cluster Showing Single Molecule Magnet Behavior*, Inorg. Chem. **47**, 6581 (2008)
- [C1.5:4] \* ‡ A. Bhunia, P.W. Roesky, Y. Lan, G.E. Kostakis, and A.K. Powell, *Salen-Based Infinite Coordination Polymers of Nickel and Copper*, Inorg. Chem. **48**, 10483 (2009)
- [C1.5:5] ‡ D.T. Thielemann, I. Fernández, and P.W. Roesky, *New Amino Acid Ligated Yttrium Hydroxy Clusters*, Dalton Trans. **39**, 6661 (2010)
- [C1.5:6] B. Murugesapandian and P.W. Roesky, *Sodium and Potassium Compounds of  $[(\eta^6\text{-benzenecarboxylate})\text{Cr}(\text{CO})_3]$  and  $[(\eta^6\text{-1,4-benzenedicarboxylate})\text{Cr}(\text{CO})_3]$* , Dalton Trans. **39**, 9598 (2010)
- [C1.5:7] C.P. Hauser, D.T. Thielemann, M. Adlung, C. Wickleder, P.W. Roesky, C.K. Weiss, and K. Landfester, *Luminescent polymeric dispersions and films based on oligonuclear lanthanide clusters*, Macromol. Chem. Phys. **212**, 286 (2011)
- [C1.5:8] B. Murugesapandian and P.W. Roesky, *Hydrogen bonding networks in  $[\eta^6\text{-arene})\text{Cr}(\text{CO})_3]$  complexes*, Heteroatom Chem. **22**, 294 (2011)
- [C1.5:9] B. Murugesapandian and P.W. Roesky, *Coordination Polymers of Zinc with  $(\eta^6\text{-Benzene carboxylate})\text{Cr}_3(\text{CO})_6$* , Inorg. Chem. **50**, 1698 (2011)
- [C1.5:10] \* P.W. Roesky, A. Bhunia, Y. Lan, A.K. Powell, and S. Kureti, *Salen-Based Metal Organic Frameworks of Nickel and the Lanthanides*, Chem. Commun. **47**, 2035 (2011)
- [C1.5:11] B. Murugesapandian and P.W. Roesky, *Synthesis and Structures of Cadmium(II) Complexes with  $(\eta^6\text{-Benzene carboxylate})\text{Cr}_3(\text{CO})_6$* , Eur. J. Inorg. Chem. 4103 (2011)
- [C1.5:12] \* A. Bhunia, Y. Lan, V. Mereacre, M.T. Gamer, A.K. Powell, and P.W. Roesky, *Salen-Based Coordination Polymers of Iron and the Rare Earth Elements*, Inorg. Chem. **50**, 12697 (2011)
- [C1.5:13] \* D.T. Thielemann, M. Klinger, T. Wolf, Y. Lan, W. Wernsdorfer, M. Busse, P.W. Roesky, A.N. Unterreiner, A.K. Powell, P.C. Junk, and G.B. Deacon, *Novel Lanthanide Based Polymeric Chains and Corresponding Ultrafast Dynamics in Solution*, Inorg. Chem. **50**, 11990 (2011)
- [C1.5:14] B. Murugesapandian and P.W. Roesky, *Synthesis and Structure of Lead(II) Complexes of  $(\eta^6\text{-Benzene carboxylato})\text{Cr}_3(\text{CO})_6$* , Eur. J. Inorg. Chem., DOI: 10.1002/ejic.201100948 (2011)

**C1.6 ‘Generation and Applications of New Nano-Structured Materials: Novel Chiral Lanthanides-C<sub>60</sub> Buckminster Fullerene Clusters’ (S. Bräse, P. Roesky)**

- [C1.6:1] P. Pierrat, C. Réthoré, T. Muller, and S. Bräse, *Design and Efficient Synthesis of Fullerene Bismalonates as Building Blocks for Metal Organic Frameworks*, *Synlett.* 1706 (2008)
- [C1.6:2] P. Pierrat, S. Vanderheiden, T. Muller, and S. Bräse, *Functionalization of Hexakis Methanofullerene Malonate Crown-Ethers: Promising Octahedral Building Blocks for Molecular Networks*, *Chem. Commun.* 1748 (2009)
- [C1.6:3] P. Pierrat, C. Réthoré, T. Muller, and S. Bräse, *Di- and Dodeca-Mitsunobu Reactions on C<sub>60</sub> Derivatives: Post-Functionalization of Fullerene Mono- and Hexakis-Adducts*, *Chem. Eur. J.* **15**, 11458 (2009)
- [C1.6:4] \* S.N. Konchenko, N.A. Pushkarevsky, M.T. Gamer, R. Köppe, H. Schnöckel, and P.W. Roesky, *[{( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>Sm}]<sub>4</sub>P<sub>8</sub>*: A Molecular Polyphosphide of the Rare Earth Elements, *J. Am. Chem. Soc.* **131**, 5740 (2009)
- [C1.6:5] \* A.J. Inglis, P. Pierrat, T. Muller, S. Bräse, and C. Barner-Kowollik, *Well-Defined Star Shaped Polymer-Fullerene Hybrids via Click Chemistry*, *Soft Matter* **6**, 82 (2010)

## **Project C3 ,Properties of Molecule Based Nanostructures'**

### **C3.2 ,Frequency and Time-Domain Electronic Spectroscopy of Isolated Clusters and Carbon Nanotubes' (M. Kappes, A. Unterreiner)**

- [C3.2:1] B. Concina, M. Neumaier, O. Hampe, and M. Kappes, *Photodetachment of Fullerene Monoanions and Dianions in a Penning Trap: Probes of Delayed Electron Emission and Associated Activation Barriers*, Int. J. of Mass Spectrom. **252**, 110 (2006)
- [C3.2:2] O. Kiowski, S. Lebedkin, and M.M. Kappes, *Photoluminescence microscopy of as-grown individual single-walled carbon nanotubes on Si/SiO<sub>2</sub> substrates*, phys. stat. sol. (b) **243**, 3122 (2006)
- [C3.2:3] \* K. Arnold, F. Hennrich, R. Krupke, S. Lebedkin, and M.M. Kappes, *Length separation studies of single walled carbon nanotube dispersions*, phys. stat. sol. (b) **243**, 3073 (2006)
- [C3.2:4] S. Lebedkin, K. Arnold, O. Kiowski, F. Hennrich, and M. Kappes, *Raman Study of Individually Dispersed Single-Walled Carbon Nanotubes under Pressure*, Phys. Rev. B **73**, 094106 (2006)
- [C3.2:5] ‡ X.-B. Wang, H.-K. Woo, X. Huang, M. Kappes, and L.-S. Wang, *Direct Experimental Probe of the Onsite Coulomb Repulsion in the Doubly Charged Fullerene Anion C<sub>70</sub><sup>2-</sup>*, Phys. Rev. Lett. **96**, 143002 (2006)
- [C3.2:6] \* O. Ehrler, J.-P. Yang, C. Hättig, A.-N. Unterreiner, H. Hippler, and M. Kappes, *Femtosecond Pump-probe Photoelectron Spectroscopy of Isolated C<sub>60</sub> Negative Ions*, J. Chem. Phys. **125**, 074312 (2006)
- [C3.2:7] \* T.S. Balaban, M.C. Balaban, S. Malik, F. Hennrich, R. Fischer, H. Rösner and M. Kappes, *Polyacetylation of Single Walled Carbon Nanotubes under Friedel-Crafts Conditions: An Efficient Method for Functionalizing, Purifying, Decorating and Linking Carbon Allotropes*, Adv. Mat. **18**, 2763 (2006)
- [C3.2:8] ‡ N. Mirsaleh-Kohan, S. Ard, A.A. Tuinman, R.N. Compton, P. Weis, and M. Kappes, *Collisional Dissociation of Salt-Cluster Dianions*, Chem. Phys. **329**, 239 (2006)
- [C3.2:9] ‡ S. Giordani, S. Bergin, V. Nicolosi, S. Lebedkin, M. Kappes, W. Blau, and J. Coleman, *Debundling of Single-Walled Nanotubes by Dilution: Observation of Large Populations of Individual Nanotubes in Amide Solvent Dispersions*, J. Phys. Chem B **110**, 15708 (2006)
- [C3.2:10] \* F. Hennrich, S. Lebedkin, K. Arnold, J. Rojas, T. Koch, T. Schimmel, R. Krupke, and M. Kappes, *The mechanism of cavitation-induced scission of single-walled carbon nanotubes*, J. Phys. Chem. B **111**, 1932 (2007)
- [C3.2:11] \* O. Kiowski, S. Lebedkin, F. Hennrich, S. Malik, H. Roesner, K. Arnold, C. Suergers, and M. Kappes, *Photoluminescence microscopy of carbon nanotubes grown by chemical vapor deposition: influence of external dielectric screening on optical transition energies*, Phys. Rev. B **75**, 075421 (2007)
- [C3.2:12] ‡ X.-B. Wang, H.-K. Woo, J. Yang, M. Kappes, and L.-S. Wang, *Photoelectron Spectroscopy of Singly and Doubly Charged Higher Fullerenes at Low Temperatures: C<sub>76</sub><sup>-</sup>, C<sub>78</sub><sup>-</sup>, C<sub>84</sub><sup>-</sup> and C<sub>76</sub><sup>2-</sup>, C<sub>78</sub><sup>2-</sup>, C<sub>84</sub><sup>2-</sup>*, J. Phys. Chem. C **111**, 17684 (2007)
- [C3.2:13] ‡ C.A. Kuntscher, K. Thirunavukkuarasu, A. Pekker, K. Kamaras, F. Hennrich, M. Kappes, and Y. Iwasa, *Pressure-induced phenomena in single-walled carbon nanotubes*, phys. stat. sol. (b) **244**, 3982 (2007)

- [C3.2:14] O. Kiowski, K. Arnold, S. Lebedkin, F. Hennrich, and M. Kappes, *Direct observation of deep dark excitonic states in the photoluminescence spectra of single-walled carbon nanotubes*, Phys. Rev. Lett. **99**, 237402 (2007)
- [C3.2:15] \* S. Blatt, F. Hennrich, H. von Löhneysen, M. Kappes, A. Vijayaraghavan, and R. Krupke, *Influence of Structural and Dielectric Anisotropy on the Dielectrophoresis of Single-Walled Carbon Nanotubes*, Nano Lett. **7**, 1960 (2007)
- [C3.2:16] \* J.-P. Yang, M.M. Kappes, H. Hippler, and A.N. Unterreiner, *Femtosecond Transient Absorption Spectroscopy of Single-Walled Carbon Nanotubes and Their Ultrafast Optical Switching Behavior*, Solid State Phenom. **121**, 905 (2007)
- [C3.2:17] \* S.S. Jester, O. Kiowski, S. Lebedkin, F. Hennrich, R. Fischer, N. Stürzl, J. Hawecker, and M.M. Kappes, *Combination of atomic force microscopy and photoluminescence microscopy for the investigation of individual carbon nanotubes on sapphire surfaces*, phys. stat. sol. (b) **244**, 3973 (2007)
- [C3.2:18] O. Kiowski, S. Lebedkin, F. Hennrich, and M.M. Kappes, *Single-walled carbon nanotubes show stable emission and simple photoluminescence spectra with weak excitation sidebands at cryogenic temperatures*, Phys. Rev. B **76**, 075422 (2007)
- [C3.2:19] ‡ O.T. Ehrler, J.-P. Yang, A.B. Sugiharto, A.N. Unterreiner, and M.M. Kappes, *Excited state dynamics of metastable phthalo-cyanine-tetrasulfonate tetraanions probed by pump/Probe photoelectron spectroscopy*, J. Chem. Phys. **127**, 184301 (2007)
- [C3.2:20] \* F. Hennrich, K. Arnold, S. Lebedkin, A. Quintilla, W. Wenzel, and M.M. Kappes, *Diameter sorting of carbon nanotubes by gradient centrifugation: role of endohedral water*, phys. stat. sol. (b) **244**, 3896 (2007)
- [C3.2:21] ‡ T. Hertel, V. Perebeinos, J. Crochet, K. Arnold, M. Kappes, and P. Avouris, *Intersubband decay of 1-D exciton resonances in carbon nanotubes*, Nano Lett. **8**, 87 (2008)
- [C3.2:22] ‡ R. Marquis, C. Greco, I. Sadokierska, S. Lebedkin, M.M. Kappes, T. Michel, L. Alvarez, J.-L. Sauvajol, S. Meunier, and C. Mioskowski, *Supramolecular discrimination of carbon nanotubes according to their helicity*, Nano Lett. **8**, 1830 (2008)
- [C3.2:23] ‡ X.-B. Wang, K. Matheis, I.N. Ioffe, A.A. Goryunkov, J. Yang, M.M. Kappes, and L.-S. Wang, *High Resolution and Low-Temperature Photoelectron Spectroscopy of an Oxygen-Linked Fullerene Dimer Dianion:  $C_{120}O^{2-}$* , J. Chem. Phys. **128**, 114307 (2008)
- [C3.2:24] S. Lebedkin, F. Hennrich, O. Kiowski, and M.M. Kappes, *Photophysics of carbon nanotubes in organic polymer-toluene dispersions: emission and excitation satellites and relaxation pathways*, Phys. Rev. B **77**, 165429 (2008)
- [C3.2:25] B. Concina, M. Neumaier, O. Hampe, and M.M. Kappes, *Electron emission from laser-heated fullerene dianions: Probing the repulsive Coulomb barrier*, J. Chem. Phys. **128**, 134306 (2008)
- [C3.2:26] ‡ S. Lebedkin, I. Kareev, F. Hennrich, and M.M. Kappes, *Efficient Quenching of Singlet Oxygen via Energy Transfer to Semiconducting Single-Walled Carbon Nanotubes*, J. Phys. Chem. C **112**, 16236 (2008)
- [C3.2:27] ‡ T. Gokus, A. Hartschuh, H. Harutyunyan, M. Allegrini, F. Hennrich, M. Kappes, A.A. Green, M.C. Hersam, P.T. Araujo, and A. Jorio, *Exciton decay dynamics in individual carbon nanotubes at room temperature*, Appl. Phys. Lett. **92**, 153116 (2008)

- [C3.2:28] S. Lebedkin, K. Arnold, O. Kiowski, F. Hennrich, and M. Kappes, *Interband Transition Energy Shifts in Photoluminescence of Single-Walled Carbon Nanotubes under Hydrostatic Pressure*, Proceedings of the International Winterschool on Electronic Properties of Novel Materials (IWEPNM 2005), H. Kuzmany, J. Fink, M. Mehring and S. Roth Eds., AIP Conference Proc. **786**, 124 (2006)
- [C3.2:29] O. Kiowski, K. Arnold, S. Lebedkin, F. Hennrich, and M. Kappes, *Detection of Single Carbon Nanotubes in Aqueous Dispersion via Photoluminescence*, Proceedings of the International Winterschool on Electronic Properties of Novel Materials (IWEPNM 2005), H. Kuzmany, J. Fink, M. Mehring and S. Roth Eds., AIP Conference Proc. **786**, 139 (2006)
- [C3.2:30] \* M. Oron, F. Hennrich, M. Kappes, and R. Krupke, *Correlation between Transport Measurements and Resonant Raman Spectroscopy on site-deposited Individual Carbon Nanotubes*, Proceedings of the International Winterschool on Electronic Properties of Novel Materials (IWEPNM 2005), H. Kuzmany, J. Fink, M. Mehring and S. Roth Eds., AIP Conference Proc. **786**, 574 (2006)
- [C3.2:31] \* K. Pulskamp, J.M. Woerle-Knirsch, F. Hennrich, K. Kern, and H. F. Krug, *Human lung epithelial cells show biphasic oxidative burst after single-walled carbon nanotube contact*, Carbon **45**, 2241 (2007)
- [C3.2:32] \* A. Vijayaraghavan, S. Blatt, D. Weissenberger, M. Oron-Carl, F. Hennrich, D. Gerthsen, H. Hahn, and R. Krupke, *Ultra-large-scale directed assembly of single-walled carbon nanotube devices*, Nano Lett. **7**, 1556 (2007)
- [C3.2:33] \* J. Hartig, F. Klöwer, J. Rinck, A.-N. Unterreiner, and H. Schnöckel, *Ga<sub>24</sub>Br<sub>18</sub>Se<sub>2</sub>: a highly symmetrical metalloid cluster and its one-dimensional arrangement in the crystalline state as a model for the photoconductivity of solid GaSe*, Angew. Chem. Int. Ed. **46**, 6549 (2007)
- [C3.2:34] \* O. Schalk, H. Brands, T.S. Balaban, and A.-N. Unterreiner, *Near-Infrared Excitation of the Q-band in Free Base and Zinc Tetraphenyl-porphyrins*, J. Phys. Chem. A **112**, 1719 (2008)
- [C3.2:35] \*‡ S. Wong, O. Kiowski, J. Lindner, F. Peiris, M. Thiel, M. Braun, M. Kappes, M. Wegener, G.A. Ozin, and G. v. Freymann, *Spatially localized photoluminescence at 1.5 micrometers wavelength in direct laser written 3D structures*, Adv. Mater. **20**, 1 (2008)
- [C3.2:36] ‡ K. Matheis, L. Joly, R. Antoine, F. Lépine, C. Bordas, O.T. Ehrler, A.-R. Allouche, M.M. Kappes, and P. Dugourd, *Photoelectron Spectroscopy of Gramicidin Polyanions: Competition between Delayed and Direct Emission*, J. Am. Chem. Soc. **130**, 15903 (2008)
- [C3.2:37] \*‡ A. Gerasko, E.A. Mainicheva, M.I. Naumova, M. Neumaier, M.M. Kappes, S. Lebedkin, D. Fenske, and V.P. Fedin, *Sandwich-type tetrานuclear lanthanide complexes with cucurbit[6]uril: from molecular compounds to coordination polymers*, Inorg. Chem. **47**, 8869 (2008)
- [C3.2:38] F. Hennrich, S. Lebedkin, and M.M. Kappes, *Improving separation techniques for single-walled carbon nanotubes: towards monodisperse samples*, phys. stat. sol. (b) **245**, 1951 (2008)
- [C3.2:39] ‡ X.-B. Wang, A.P. Sergeeva, X.-P. Xing, M. Massaouti, T. Karpuschkin, O. Hampe, A.I. Boldyrev, M.M. Kappes, and L.-S. Wang, *Probing the Electronic Stability of Multiply Charged Anions: the Sulfonated Pyrene Tri- and Tetra-Anions*, J. Am. Chem. Soc. **131**, 9836 (2009)
- [C3.2:40] ‡ O. Kiowski, S.-S. Jester, S. Lebedkin, Z. Jin, Y. Li, and M.M. Kappes, *Photoluminescence Spectral Imaging of Ultralong Single-Walled Carbon*

*Nanotubes: Micromanipulation-Induced Strain, Rupture and the Determination of Handedness*, Phys. Rev. B **80**, 075426 (2009)

- [C3.2:41] N. Stürzl, F. Hennrich, S. Lebedkin, and M.M. Kappes, *Near Monochiral Single-Walled Carbon Nanotube Dispersions in Organic Solvents*, J. Phys. Chem. C **113**, 14628 (2009)
- [C3.2:42] K. Moshammer, F. Hennrich, and M.M. Kappes, *Selective Suspension in Aqueous Sodium Dodecyl Sulfate According to Electronic Structure Type Allows Simple Separation of Metallic from Semiconducting Single-Walled Carbon Nanotubes*, Nano Res. **2**, 599 (2009)
- [C3.2:43] ‡ O. Hampe, M. Neumaier, A.D. Boese, J. Lemaire, G. Niedner-Schattburg, and M.M. Kappes, *Infrared multiphoton electron detachment spectroscopy of  $C_{76}^{2-}$* , J. Chem. Phys. **131**, 124306 (2009)
- [C3.2:44] ‡ C. Rensing, O.T. Ehrler, J.-P. Yang, A.-N. Unterreiner, and M.M. Kappes, *Photodissociation dynamics of  $IrBr_6^{2-}$  dianions by time-resolved photoelectron spectroscopy*, J. Chem. Phys. **130**, 234306 (2009)
- [C3.2:45] ‡ S. Kyatskaya, J.R. Galán Mascarós, L. Bogani, F. Hennrich, M. Kappes, W. Wernsdorfer, and M. Ruben, *Anchoring of rare-earth-based single-molecule magnets on single-walled carbon nanotubes*, J. Am. Chem. Soc. **131**, 15143 (2009)
- [C3.2:46] ‡ R. Marquis, K. Kulikiewicz, S. Lebedkin, M.M. Kappes, C. Mioskowski, S. Meunier, and A. Wagner, *Axially Chiral Facial Amphiphiles with a Dihydronaphthopentaphene Structure as Molecular Tweezers for SWNTs*, Chem. Eur. J. **15**, 11187 (2009)
- [C3.2:47] ‡ C.Z. Loebick, S. Derrouiche, N. Marinkovic, C. Wang, F. Hennrich, M.M. Kappes, G.L. Haller, and L.D. Pfefferle, *Effect of Manganese Addition to the Co-MCM-41 Catalyst in the Selective Synthesis of Single Wall Carbon Nanotubes*, J. Phys. Chem. C **113**, 21611 (2009)
- [C3.2:48] N. Stürzl, S. Lebedkin, S. Malik, and M.M. Kappes, *Preparation of  $^{13}C$  single-walled Carbon Nanotubes by pulsed Laser Vaporization*, phys. stat. sol. (b) **246**, 2465 (2009)
- [C3.2:49] \* A. Quintillá, F. Hennrich, S. Lebedkin, M.M. Kappes, and W. Wenzel, *Influence of endohedral water on diameter sorting of single-walled carbon nanotubes by density gradient centrifugation*, Phys. Chem. Chem. Phys. **12**, 902 (2010)
- [C3.2:50] \*‡ S. Essig, C.W. Marquardt, A. Vijayaraghavan, M. Ganzhorn, S. Dehm, F. Hennrich, F. Ou, A.A. Green, C. Scasia, F. Bonaccorso, K.-P. Bohnen, H. v. Loehneysen, M.M. Kappes, P. Ajayan, M.C. Hersam, A. Ferrari, and R. Krupke, *Phonon-assisted electroluminescence from metallic carbon nanotubes and graphene*, Nano Lett. **10**, 1589 (2010)
- [C3.2:51] \* A. Vijayaraghavan, F. Hennrich, N. Stürzl, M. Engel, M. Ganzhorn, M. Oron-Carl, C.W. Marquardt, S. Dehm, S. Lebedkin, M.M. Kappes, and R. Krupke, *Toward Single-Chirality Carbon Nanotube Device Arrays*, ACS Nano **4**, 2748 (2010)
- [C3.2:52] \* A. Stuparu, C. Stroh, F. Hennrich, and M.M. Kappes, *Dispersion of Single Walled Carbon Nanotubes using Poly(3-dodecylthiophene-2,5-diyl)*, phys. stat. sol. (b) **247**, 2653 (2010)
- [C3.2:53] ‡ J. Lindner, A.-N. Unterreiner, and P. Vöhringer, *Femtosecond spectroscopy of solvated electrons from sodium-ammonia-d3 solutions: Temperature jump versus local density jump*, J. Chem. Phys. **129**, 064514 (2008)

- [C3.2:54] O. Schalk, J.-P. Yang, A. Hertwig, H. Hippler, and A.-N. Unterreiner, *Vibrational cooling in the liquid phase studied by ultrafast investigations of cycloheptatriene*, Mol. Phys. **107**, 2159 (2009)
- [C3.2:55] O. Schalk and A.-N. Unterreiner, *The influence of rotational diffusion on transient anisotropy in ultrafast experiments*, Phys. Chem. Chem. Phys. **12**, 655 (2010)
- [C3.2:56] C. Nese and A.-N. Unterreiner, *Photochemical processes in ionic liquids on ultrafast timescales*, Phys. Chem. Chem. Phys. **12**, 1698 (2010)
- [C3.2:57] ‡ H. Palza, B. Reznik, M. Kappes, F. Hennrich, I.F.C. Naue, and M. Wilhelm, *Characterization of melt flow instabilities in polyethylene/carbon nanotube composites*, Polymer **51**, 3753 (2010)
- [C3.2:58] S. Lebedkin, C. Blum, N. Stürzl, F. Hennrich, and M. Kappes, *A low-wavenumber-extended confocal Raman microscope with very high laser excitation line discrimination*, Rev. Sci. Instr. **82**, 013705 (2011)
- [C3.2:59] \* N. Berton, F. Lemasson, J. Tittmann, N. Stürzl, F. Hennrich, M. Kappes, and M. Mayor, *Copolymer-Controlled Diameter-Selective Dispersion of Semiconducting Single-Walled Carbon Nanotubes*, Chem. Mater. **23**, 2237 (2011)
- [C3.2:60] C. Blum, N. Stuerzl, F. Hennrich, S. Lebedkin, S. Heeg, H. Dumlich, S. Reich, and M. Kappes, *Selective bundling of zig-zag single-walled carbon nanotubes*, ACS Nano **5**, 2847 (2011)
- [C3.2:61] \* F. Lemasson, J. Tittmann, F. Hennrich, N. Stürzl, S. Malik, M. Kappes, and M. Mayor, *Debundling, Selection and Release of SWNTs Using Fluorene-Based Photocleavable Polymers*, Chem. Comm. **47**, 7428 (2011)
- [C3.2:62] \* O. Hampe, T. Karpuschkin, M. Vonderach, P. Weis, Y. Yu, L. Gan, W. Klopper, and M. Kappes, *Heating a bowl of single-molecule-soup: structure and desorption energetics of water-encapsulated open-cage (60) fullerenoid anions in gas-phase*, Phys. Chem. Chem. Phys. **13**, 9818 (2011)
- [C3.2:63] \* C. Thiele, M. Engel, F. Hennrich, M. Kappes, H. v. Löhneysen, and R. Krupke, *Controlled fabrication of single-walled carbon nanotube electrodes by electron-beam induced oxidation*, Appl. Phys. Lett. **99**, 173105 (2011)
- [C3.2:64] \* H. Brands, O.T. Ehrler, M. Kappes, and A.-N. Unterreiner, *Relaxation Dynamics of Electronically Excited C<sub>60</sub><sup>-</sup> in o-Dichlorobenzene and Tetrahydrofuran Solution*, Z. Phys. Chem. **255**, 939 (2011)
- [C3.2:65] \* J. Pelka, H. Gehrke, A. Rechel, M. Kappes, F. Hennrich, C. Hartinger, and D. Marko, *DNA damaging properties of single walled carbon nanotubes in human colon carcinoma cells*, Nanotoxicology, DOI: 10.3109/17435390.2011.626536 (2011)
- [C3.2:66] \* M. Pfeiffer, N. Stürzl, C. Marquardt, M. Engel, S. Dehm, F. Hennrich, M. Kappes, U. Lemmer, and R. Krupke, *Electroluminescence from chirality-sorted (9,7)- semiconducting carbon nanotube devices*, Optics Express **19**, A1184 (2011)
- [C3.2:67] \* M. Mastronardi, F. Hennrich, E. Henderson, F. Maier-Flaig, C. Blum, J. Reichenbach, U. Lemmer, C. Kuebel, D. Wang, M. Kappes, and G. Ozin, *Preparation of Monodisperse Silicon Nanocrystals Using Density Gradient Ultracentrifugation*, J. Am. Chem. Soc. **133**, 11928 (2011)
- [C3.2:68] \* T. Wolf, J. Fischer, M. Wegener, and A.-N. Unterreiner, *Pump-probe spectroscopy on photoinitiators for stimulated-emission-depletion optical lithography*, Opt. Lett. **36**, 3188 (2011)

- [C3.2:69] O. Schalk and A. –N. Unterreiner, *Transient anisotropy in degenerate systems: A semi-classical approach*, Z. Phys. Chem. **225**, 927 (2011)
- [C3.2:70] \* ‡ D. Thielemann, M. Klinger, T. Wolf, Y. Lan, W. Wernsdorfer, M. Busse, P. Roesky, A.-N. Unterreiner, A. Powell, P. Junk, and G. Deacon, *Novel Lanthanide-Based Polymeric Chains and Corresponding Ultrafast Dynamics in Solution*, Inorg. Chem., DOI: 10.1021/ic201157m (2011)
- [C3.2:71] \* F. Hennrich, M. Kappes, M. Klinger, and A.-N. Unterreiner, *Ultrafast Dynamics of the First Excited State of Quasi Monodispersed Single-Walled (9,7) Carbon Nanotubes*, J. Phys. Chem. C **115**, 23711 (2011)

### C3.3 ‘Computation of Electronic and Intermolecular Interactions’ (W. Klopper)

- [C3.3:1] H. Fliegl, C. Hättig, and W. Klopper, *Coupled-cluster response theory with linear- $r_{12}$  corrections: The CC2-R12 model for excitation energies*, J. Chem. Phys. **124**, 044112 (2006)
- [C3.3:2] \* C.E. Anson, W. Klopper, J.-S. Li, L. Ponikiewski, and A. Rothenberger, *A close look at short C-CH<sub>3</sub>...potassium contacts: Synthetic and theoretical investigations of [M<sub>2</sub>Co<sub>2</sub>(μ<sub>3</sub>-OtBu)<sub>2</sub>(μ<sub>2</sub>-OtBu)<sub>4</sub>(thf)<sub>n</sub>] (M = Na, K, Rb, thf = tetrahydrofuran)*, Chem. Eur. J. **12**, 2032 (2006)
- [C3.3:3] H. Fliegl, C. Hättig, and W. Klopper, *Inclusion of the (T) triples correction into the linear- $r_{12}$  corrected coupled-cluster model CCSD(R12)*, Int. J. Quantum Chem. **106**, 2306 (2006)
- [C3.3:4] ‡ H.-J. Himmel, O. Hübner, W. Klopper, and L. Manceron, *Cleavage of the N<sub>2</sub> triple bond by the Ti dimer: A route to molecular materials for dinitrogen activation?*, Angew. Chem. Int. Ed. **45**, 2799 (2006); *Spaltung der N<sub>2</sub>-Dreifachbindung durch Ti<sub>2</sub>: ein Weg zu molekularen Materialien für die N<sub>2</sub>-Aktivierung?*, Angew. Chem. **118**, 2865 (2006)
- [C3.3:5] ‡ H.-J. Himmel, O. Hübner, F.A. Bischoff, W. Klopper, and L. Manceron, *Reactivity of titanium dimer and molecular nitrogen in rare gas matrices. Vibrational and electronic spectra and structure of Ti<sub>2</sub>N<sub>2</sub>*, Phys. Chem. Chem. Phys. **8**, 2000 (2006)
- [C3.3:6] ‡ T. Helgaker, A.C. Hennum, and W. Klopper, *A second-quantization framework for the unified treatment of relativistic and nonrelativistic molecular perturbations by response theory*, J. Chem. Phys. **125**, 024102 (2006)
- [C3.3:7] ‡ W. Klopper, F.R. Manby, S. Ten-no, and E.F. Valeev, *R12 methods in explicitly correlated molecular electronic structure theory*, Int. Rev. Phys. Chem. **25**, 427 (2006)
- [C3.3:8] ‡ M. Heckert, M. Kállay, D.P. Tew, W. Klopper, and J. Gauss, *Basis-set extrapolation techniques for the accurate calculation of molecular equilibrium geometries using coupled-cluster theory*, J. Chem. Phys. **125**, 044108 (2006)
- [C3.3:9] H. Fliegl, A. Glöß, O. Welz, M. Olzmann, and W. Klopper, *Accurate computational determination of the binding energy of the SO<sub>3</sub>-H<sub>2</sub>O complex*, J. Chem. Phys. **125**, 054312 (2006)
- [C3.3:10] O. Hübner, M. Fichtner, and W. Klopper, *Comment on ‘A theoretical study of nanoporous organic molecules for hydrogen storage’ [Micropor. Mesopor. Mater. 89 (2006) 138]*, Micropor. Mesopor. Mater. **94**, 371 (2006)
- [C3.3:11] D.P. Tew and W. Klopper, *A comparison of linear and nonlinear correlation factors for basis set limit Møller-Plesset second order binding energies and structures of He<sub>2</sub>, Be<sub>2</sub> and Ne<sub>2</sub>*, J. Chem. Phys. **125**, 094302 (2006)
- [C3.3:12] M.K. Armbruster, W. Klopper, and F. Weigend, *Basis-set extensions for two-component spin-orbit treatments of heavy elements*, Phys. Chem. Chem. Phys. **8**, 4862 (2006)
- [C3.3:13] ‡ R.A. Bachorz, W. Klopper, and M. Gutowski, *Coupled-cluster and explicitly correlated perturbation-theory calculations of the uracil anion*, J. Chem. Phys. **126**, 085101 (2007)
- [C3.3:14] \* F.A. Bischoff, O. Hübner, W. Klopper, L. Schnelzer, B. Pilawa, M. Horvatić, and C. Berthier, *Density-functional calculation of the quadrupole splitting in the <sup>23</sup>Na NMR spectrum of the ferric wheel Na@Fe<sub>6</sub>(tea)<sub>6</sub><sup>+</sup> for various broken-symmetry states of the Heisenberg spin model*, Eur. Phys. J. B **55**, 229 (2007)

- [C3.3:15] O. Hübner and W. Klopper, *Interaction of dihydrogen with small and light molecules*, J. Phys. Chem. A **111**, 2426 (2007)
- [C3.3:16] ‡ D.P. Tew, W. Klopper, and T. Helgaker, *Electron correlation: The many-body problem at the heart of chemistry*, J. Comput. Chem. **28**, 1307 (2007)
- [C3.3:17] O. Hübner, K. Fink, and W. Klopper, *The spin coupling in the diiron complex [Fe<sub>2</sub>(hppta)(H<sub>2</sub>O)<sub>3</sub>Cl]*, Phys. Chem. Chem. Phys. **9**, 1911 (2007)
- [C3.3:18] ‡ D.P. Tew, W. Klopper, C. Neiss, and C. Hättig, *Quintuple- $\zeta$  coupled-cluster correlation energies with triple- $\zeta$  basis sets*, Phys. Chem. Chem. Phys. **9**, 1921 (2007)
- [C3.3:19] ‡ R. Leist, J.A. Frey, P. Ottiger, H.-M. Frey, S. Leutwyler, R.A. Bachorz, and W. Klopper, *Nucleobase-fluorobenzene interactions: Hydrogen bonding wins over  $\pi$ -stacking*, Angew. Chem. Int. Ed. **46**, 7449 (2007)
- [C3.3:20] ‡ D.P. Tew, W. Klopper, and F.R. Manby, *The weak orthogonality functional in explicitly correlated pair theories*, J. Chem. Phys. **127**, 174105 (2007)
- [C3.3:21] ‡ A.D. Boese, J.M.L. Martin, and W. Klopper, *Basis set limit coupled cluster study of H-bonded systems and assessment of more approximate methods*, J. Phys. Chem. A **111**, 11122 (2007)
- [C3.3:22] ‡ D.P. Tew, W. Klopper, M. Heckert, and J. Gauss, *Basis set limit CCSD(T) harmonic vibrational frequencies*, J. Phys. Chem. A **111**, 11242 (2007)
- [C3.3:23] T. Pankewitz and W. Klopper, *Ab initio modeling of methanol interaction with single-walled carbon nanotubes*, J. Phys. Chem. C **111**, 18917 (2007)
- [C3.3:24] ‡ E. Klontzas, A. Mavrandonakis, G.E. Froudakis, Y. Carissan, and W. Klopper, *Molecular hydrogen interaction with IRMOF-1: A multiscale theoretical study*, J. Phys. Chem. C **111**, 13635 (2007)
- [C3.3:25] A. Mavrandonakis and W. Klopper, *Comment on 'Kinetics and Mechanistic Model for Hydrogen Spillover on Bridged Metal-Organic Frameworks'*, J. Phys. Chem. C **112**, 3152 (2008)
- [C3.3:26] ‡ D.P. Tew, W. Klopper, and C. Hättig, *A diagonal orbital-invariant explicitly-correlated coupled-cluster method*, Chem. Phys. Lett. **452**, 326 (2008)
- [C3.3:27] ‡ M.K. Armbruster, F. Weigend, C. van Wüllen, and W. Klopper, *Self-consistent treatment of spin-orbit interactions with efficient Hartree-Fock and density functional methods*, Phys. Chem. Chem. Phys. **10**, 1748 (2008)
- [C3.3:28] T. Wedel, T. Gehring, J. Podlech, E. Kordel, A. Bihlmeier, and W. Klopper, *Nucleophilic additions to alkylidene bis(sulfoxides) – stereoelectronic effects in vinyl sulfoxides*, Chem. Eur. J. **14**, 4631 (2008)
- [C3.3:29] ‡ R.A. Bachorz, F.A. Bischoff, S. Höfener, W. Klopper, P. Ottiger, R. Leist, J.A. Frey, and S. Leutwyler, *Scope and limitations of the SCS-MP2 method for stacking and hydrogen bonding interactions*, Phys. Chem. Chem. Phys. **10**, 2758 (2008)
- [C3.3:30] S. Höfener, F.A. Bischoff, A. Glöß, and W. Klopper, *Slater-type geminals in explicitly-correlated perturbation theory: Application to n-alkanols and analysis of errors and basis-set requirements*, Phys. Chem. Chem. Phys. **10**, 3390 (2008)
- [C3.3:31] A. Mavrandonakis and W. Klopper, *First-principles study of single and multiple dihydrogen interaction with Li containing benzene molecules*, J. Phys. Chem. C **112**, 11580 (2008)
- [C3.3:32] ‡ R.A. Bachorz, W. Klopper, M. Gutowski, X. Li, and K.H. Bowen, *Photoelectron spectrum of valence anions of uracil and first-principles calculations of excess electron binding energies*, J. Chem. Phys. **129**, 054309 (2008)

- [C3.3:33] ‡ S.N. Eustis, D. Radisic, K.H. Bowen, R.A. Bachorz, M. Haranczyk, G.K. Schenter, and M. Gutowski, *Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia*, *Science* **319**, 936 (2008)
- [C3.3:34] F.A. Bischoff, S. Höfener, A. Glöß, and W. Klopper, *Explicitly-correlated second-order perturbation theory calculations on molecules containing heavy main-group elements*, *Theor. Chem. Acc.* **121**, 11 (2008)
- [C3.3:35] A. Bihlmeier, D.P. Tew, and W. Klopper, *Low energy hydrogenation products of extended  $\pi$  systems  $C_nH_{2x}$ : A DFT search strategy, benchmarked against CCSD(T) and applied to  $C_{60}$* , *J. Chem. Phys.* **129**, 114303 (2008)
- [C3.3:36] W. Klopper, D.P. Tew, N. González-García, and M. Olzmann, *Heat of formation of the  $HOSO_2$  radical from accurate quantum chemical calculations*, *J. Chem. Phys.* **129**, 114308 (2008)
- [C3.3:37] T. Pankewitz and W. Klopper, *Theoretical investigation of equilibrium and transition state structures, binding energies and barrier heights of water-encapsulated open-cage [59]fullerenone complexes*, *Chem. Phys. Lett.* **465**, 48 (2008)
- [C3.3:38] \* T. Pankewitz, W. Klopper, P. Henke, and H. Schnöckel, *Isomeric  $Al_4R_4$ ,  $Mg_2R_2$  species and oligomerisation products: Investigation of Al-Al and Mg-Mg  $\sigma$ -bonding*, *Eur. J. Inorg. Chem.* 4879 (2008)
- [C3.3:39] ‡ S. Taubert, D. Sundholm, J. Jusélius, W. Klopper, and H. Fliegl, *Calculation of magnetically induced currents in hydrocarbon nanorings*, *J. Phys. Chem. A* **112**, 13584 (2008)
- [C3.3:40] ‡ K.D. Vogiatzis, A. Mavrandonakis, W. Klopper, and G.E. Froudakis, *Ab initio study of the interactions between  $CO_2$  and N-containing organic heterocycles*, *ChemPhysChem* **10**, 374 (2009)
- [C3.3:41] A. Bihlmeier and W. Klopper, *Hydrides and dimers of  $C_{58}$  fullerenes: Structures and stabilities*, *Phys. Chem. Chem. Phys.* **11**, 1050 (2009)
- [C3.3:42] ‡ P. Ottinger, C. Pfaffen, R. Leist, S. Leutwyler, R.A. Bachorz, and W. Klopper, *Strong N-H... $\pi$  hydrogen bonding in amide-benzene interactions*, *J. Phys. Chem. B* **113**, 2937 (2009)
- [C3.3:43] \* D. Löffler, N. Bajales, M. Cudaj, P. Weis, S. Lebedkin, A. Bihlmeier, D.P. Tew, W. Klopper, A. Böttcher, and M.M. Kappes, *Non-IPR  $C_{60}$  solids*, *J. Chem. Phys.* **130**, 164705 (2009)
- [C3.3:44] \* H. Fliegl, K. Fink, W. Klopper, C.E. Anson, A.K. Powell, and R. Clérac, *Ab initio study of the magnetic exchange coupling constants of a structural model [ $CaMn_3^{III}Mn^{II}$ ] of the oxygen evolving center in photosystem II*, *Phys. Chem. Chem. Phys.* **11**, 3900 (2009)
- [C3.3:45] \* R. Abuhmaiera, Y. Lan, A.M. Ako, G.E. Kostakis, A. Mavrandonakis, W. Klopper, R. Clérac, C.E. Anson, and A.K. Powell, *One-dimensional Cu(II) coordination polymers: Tuning the structure by modulating the “carboxylate arm” lengths of polycarboxylate ligands*, *CrystEngComm* **11**, 1089 (2009)
- [C3.3:46] ‡ H. Fliegl, D. Sundholm, S. Taubert, J. Jusélius, and W. Klopper, *Magnetically induced current densities in aromatic, antiaromatic, homoaromatic, and nonaromatic hydrocarbons*, *J. Phys. Chem. A* **113**, 8668 (2009)
- [C3.3:47] \* P. Henke, T. Pankewitz, W. Klopper, F. Breher, and H. Schnöckel, *Snapshots of the AlAl- $\sigma$ -bond formation starting from  $\{AlR_2\}$  units: Experimental and computational observations*, *Angew. Chem. Int. Ed.* **48**, 8141 (2009); *Momentaufnahmen bei der Bildung einer AlAl- $\sigma$ -Bindung aus „AlR<sub>2</sub>“-Einheiten*.

*Experimentelle und quantenchemische Befunde*, Angew. Chem. **121**, 8285 (2009)

- [C3.3:48] \* G.E. Kostakis, A. Mavrandonakis, G. Abbas, W. Klopper, D. Schooss, S. Lebedkin, Y. Lan, and A.K. Powell, *An in-depth study on hydrogen-bonded 3-D frameworks possessing hydrophobic layers and hydrophilic pillars*, CrystEngComm **11**, 2480 (2009)
- [C3.3:49] ‡ I.S.K. Kerkines, I.D. Petsalakis, G. Theodorakopoulos, and W. Klopper, *Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods*, J. Chem. Phys. **131**, 224315 (2009)
- [C3.3:50] \* A. Eichhöfer, J. Olkowska-Oetzel, D. Fenske, K. Fink, V. Mereacre, A.K. Powell, and G. Buth, *Synthesis and structure of an “iron-doped” copper selenide cluster molecule:  $[Cu_{30}Fe_2Se_6(SePh)_{24}(dppm)_4]$* , Inorg. Chem. **48**, 8977 (2009)
- [C3.3:51] ‡ W. Klopper, R.A. Bachorz, D.P. Tew, and C. Hättig, *Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne*, Phys. Rev. A **81**, 022503 (2010)
- [C3.3:52] F.A. Bischoff and W. Klopper, *Second-order electron-correlation and self-consistent spin-orbit treatment of heavy molecules at the basis-set limit*, J. Chem. Phys. **132**, 094108 (2010)
- [C3.3:53] ‡ F.A. Bischoff, E.F. Valeev, W. Klopper, and C.L. Janssen, *Scalar relativistic explicitly correlated R12 methods*, J. Chem. Phys. **132**, 214104 (2010)
- [C3.3:54] ‡ C. Pfaffen, H.-M. Frey, P. Ottinger, S. Leutwyler, R.A. Bachorz, and W. Klopper, *Large-amplitude vibrations of an N-H... $\pi$  hydrogen bonded cis-amide–benzene complex*, Phys. Chem. Chem. Phys. **12**, 8208 (2010)
- [C3.3:55] \*‡ V.A. Soloshonok, T. Ono, H. Ueki, N. Vanthuyne, T.S. Balaban, J. Bürck, H. Fliegl, W. Klopper, J.-V. Naubron, T.T.T. Bui, A.F. Drake, and C. Roussel, *Ridge-tile-like chiral topology: Synthesis, resolution, and complete chiroptical characterization of enantiomers of edge-sharing binuclear square planar complexes of Ni(II) bearing achiral ligands*, J. Am. Chem. Soc. **132**, 10477 (2010)
- [C3.3:56] \* D. Nied, R. Köppe, W. Klopper, H. Schnöckel, and F. Breher, *Synthesis of a pentasilapropellane: Exploring the nature of a stretched silicon-silicon bond in a nonclassical molecule*, J. Am. Chem. Soc. **132**, 10264 (2010)
- [C3.3:57] T. Pankewitz and W. Klopper, *Interaction of the alcohol molecules methanol and ethanol with single-walled carbon nanotubes – A computational study*, Chem. Phys. Lett. **498**, 345 (2010)
- [C3.3:58] \* S. Ay, R.E. Ziegert, H. Zhang, M. Nieger, K. Rissanen, K. Fink, A. Kubas, R.M. Gschwind, and S. Bräse, *NMR-spectroscopic and solid-state investigations of cometal-free asymmetric conjugate addition: A dinuclear paracyclophaneimine zinc methyl complex*, J. Am. Chem. Soc. **132**, 12899 (2010)
- [C3.3:59] ‡ Q.Y. Zhang, T. Pankewitz, S.M. Liu, W. Klopper, and L.B. Gan, *Switchable open-cage fullerene for water encapsulation*, Angew. Chem. Int. Ed. **49**, 9935 (2010)
- [C3.3:60] ‡ A.D. Boese, G. Jansen, M. Torheyden, S. Höfener, and W. Klopper, *Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers ammonia, water, and hydrogen fluoride*, Phys. Chem. Chem. Phys. **13**, 1230 (2011)
- [C3.3:61] ‡ K.D. Vogiatzis, E.C. Barnes, and W. Klopper, *Interference-corrected explicitly-correlated second-order perturbation theory*, Chem. Phys. Lett. **503**, 157 (2011)

- [C3.3:62] \* C. Schenk, A. Kracke, K. Fink, A. Kubas, W. Klopper, M. Neumaier, H. Schnöckel, and A. Schnepf, *The formal combination of three singlet biradicaloid entities to a singlet hexaradicaloid metalloid Ge<sub>14</sub>[Si(SiMe<sub>3</sub>)<sub>3</sub>]<sub>5</sub>[Li(THF)<sub>2</sub>]<sub>3</sub> cluster*, J. Am. Chem. Soc. **133**, 2518 (2011)
- [C3.3:63] \* M. Klipfel, C. Réthoré, T. Muller, S. Bräse, and W. Klopper, *Genetic algorithm density functional theory study of crown ether-dibenzylammonium [2]pseudorotaxanes*, Comput. Theor. Chem. **966**, 186 (2011)
- [C3.3:64] \* O. Hampe, T. Karpuschkin, M. Vonderach, P. Weis, Y.M. Yu, L.B. Gan, W. Klopper, and M.M. Kappes, *Heating a bowl of single-molecule-soup: Structure and desorption energetics of water-encapsulated open-cage [60]fullerenoid anions in the gas-phase*, Phys. Chem. Chem. Phys. **13**, 9818 (2011)
- [C3.3:65] ‡ R.A. Bachorz, F.A. Bischoff, A. Glöß, C. Hättig, S. Höfener, W. Klopper, and D.P. Tew, *The MP2-F12 method in the Turbomole program package*, J. Comput. Chem. **32**, 2492 (2011)
- [C3.3:66] ‡ W. Klopper, A.M. Teale, S. Coriani, T.B. Pedersen, and T. Helgaker, *Spin flipping in ring-coupled-cluster-doubles theory*, Chem. Phys. Lett. **510**, 147 (2011)
- [C3.3:67] A. Bihlmeier, *Derivatives and dimers of C<sub>50</sub>-D<sub>5h</sub> and C<sub>50</sub>-D<sub>3</sub>: A comparison of two closely related but quite differently behaving fullerenes*, J. Chem. Phys. **135**, 044310 (2011)
- [C3.3:68] ‡ A. Baldes, W. Klopper, J. Šimunek, J. Noga, and F. Weigend, *Acceleration of self-consistent-field convergence by combining conventional diagonalization and a diagonalization-free procedure*, J. Comput. Chem. **32**, 3129 (2011)
- [C3.3:69] K.D. Vogiatzis, W. Klopper, A. Mavrandonakis, and K. Fink, *Magnetic properties of paddlewheels and trinuclear clusters with exposed metal sites*, ChemPhysChem **12**, 3307 (2011)

### C3.6 ,Theory of Transport through Single Molecules' (G. Schön, F. Pauly)

- [C3.6:1] ‡ H. van Zalinge, D.J. Schiffrin, A.D. Bates, E.B. Starikov, W. Wenzel, and R.J. Nichols, *Variable-temperature measurements of the single-molecule conductance of double-stranded DNA*, Angew. Chem. Int. Ed. **45**, 5499 (2006)
- [C3.6:2] ‡ T. Tanabe, E.B. Starikov, K. Noda, and M. Saito, *Resonant neutral-particle emission after collisions of electrons with base-stacked oligonucleotide cations in a storage ring*, Chem. Phys. Lett. **430**, 380 (2006)
- [C3.6:3] ‡ E.B. Starikov, T. Fujita, H. Watanabe, Y. Sengoku, S. Tanaka, and W. Wenzel, *Effects of molecular motion on charge transfer/transport through DNA duplexes with and without base pair mismatch*, Mol. Simulat. **32**, 759 (2006)
- [C3.6:4] ‡ E.B. Starikov, S. Tanaka, N. Kurita, Y. Sengoku, T. Natsume, A. Quintilla, and W. Wenzel, *Ballistic conductance for all-atom models of native and chemically modified DNA: a review of Kubo-formula-based approach*, In: Modern Methods for Theoretical Physical Chemistry of Biopolymers, Eds. E.B. Starikov, J.P. Lewis, and S. Tanaka (Elsevier, Amsterdam, 2006)
- [C3.6:5] \* ‡ C. Romeike, M. Wegewijs, W. Wenzel, M. Ruben, and H. Schoeller, *Charge-induced modulation of magnetic interactions in 2x2 metallo-organic grid-complex*, Int. J. Quantum Chem. **106**, 994 (2006)
- [C3.6:6] \* ‡ C. Romeike, M. Wegewijs, W. Wenzel, M. Ruben, and H. Schoeller, *Charge-switchable molecular magnet and spin-blockade of tunneling*, Phys. Rev. B **75**, 064404 (2007)
- [C3.6:7] B.B. Schmidt, M.H. Hettler, and G. Schön, *Influence of vibrational modes on the electronic properties of DNA*, Phys. Rev. B **75**, 115125 (2007)
- [C3.6:8] \* B.B. Schmidt, E.B. Starikov, M.H. Hettler, and W. Wenzel, *Vibrations in DNA: Their Influence on Transport*, in Charge migration in DNA - Physics, Chemistry and Biology Perspectives, Springer 2007 (ISBN 354-072-493-1), pp. 249-262
- [C3.6:9] ‡ J.K. Viljas and J.C. Cuevas, *Role of electronic structure in photo-assisted transport through atomic-sized contacts*, Phys. Rev. B **75**, 075406 (2007)
- [C3.6:10] ‡ J.K. Viljas, F. Pauly, and J.C. Cuevas, *Photoconductance of organic single-molecule contacts*, Phys. Rev. B **76**, 033403 (2007)
- [C3.6:11] ‡ S. Wohlthat, F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Ab initio study of charge transport through single oxygen molecules in atomic aluminum contacts*, Phys. Rev. B **76**, 075413 (2007)
- [C3.6:12] \* ‡ F. Pauly, J.K. Viljas, U. Huniar, M. Häfner, S. Wohlthat, M. Bürkle, J.C. Cuevas, and G. Schön, *Cluster-based density-functional approach to quantum transport through molecular and atomic contacts*, New J. Phys. **10**, 125019 (2008)
- [C3.6:13] ‡ M. Kiguchi, O. Tal, S. Wohlthat, F. Pauly, M. Krieger, D. Djukic, J.C. Cuevas, and J.M. van Ruitenbeek, *Highly conductive molecular junctions based on direct binding of benzene to platinum*, Phys. Rev. Lett. **101**, 046801 (2008)
- [C3.6:14] ‡ S. Wohlthat, F. Pauly, and J.R. Reimers, *The conduction properties of  $\alpha,\omega$ -diaminoalkanes and hydrazine bridging gold electrodes*, Chem. Phys. Lett. **454**, 284 (2008)
- [C3.6:15] ‡ F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Density-functional study of tilt-angle and temperature-dependent conductance in biphenyl-dithiol single-molecule contacts*, Phys. Rev. B **77**, 155312 (2008)

- [C3.6:16] ‡ F. Pauly, J.K. Viljas, and J.C. Cuevas, *Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives*, Phys. Rev. B **78**, 035315 (2008)
- [C3.6:17] ‡ S. Wohlthat, F. Pauly, and J.R. Reimers, *Two-dimensional, phenanthroline-based, extended  $\pi$ -conjugated molecules for single-molecule conduction*, J. Phys-Condens. Mat. **20**, 295208 (2008)
- [C3.6:18] ‡ J.K. Viljas, F. Pauly, and J.C. Cuevas, *Modeling elastic and photoassisted transport in organic molecular wires: Length dependence and current-voltage characteristics*, Phys. Rev. B **77**, 155119 (2008)
- [C3.6:19] ‡ A.V. Danilov, P. Hedegard, D.S. Golubev, T. Bjornholm, and S.E. Kubatkin, *Nanoelectromechanical switch operating by tunneling of an entire C<sub>60</sub> molecule*, Nano Lett. **8**, 2393 (2008)
- [C3.6:20] ‡ J.J. Kwiatkowski, J. Nelson, H. Li, J.L. Bredas, W. Wenzel, and C. Lennartz, *Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq3)*, Phys. Chem. Chem. Phys. **10**, 1852 (2008)
- [C3.6:21] B.B. Schmidt, M.H. Hettler, and G. Schön, *Non-equilibrium polaron hopping transport through DNA*, Phys. Rev. B **77**, 165337 (2008)
- [C3.6:22] E.B. Starikov, A. Quintilla, K.H. Lee, and W. Wenzel, *Conformational dependence of DNA ballistic conductivity*, J. Chem. Phys. **129**, 131101 (2008)
- [C3.6:23] ‡ E.B. Starikov, A. Quintilla, C. Nganou, K.H. Lee, G. Cuniberti, and W. Wenzel, *Single-molecule DNA conductance in water solutions: Role of DNA low-frequency dynamics*, Chem. Phys. Lett. **467**, 369 (2009)
- [C3.6:24] B.B. Schmidt, M.H. Hettler, and G. Schön, *Charge correlations in polaron hopping through molecules*, Phys. Rev. B **82**, 155113 (2010)
- [C3.6:25] ‡ L.A. Zotti, T. Kirchner, J.C. Cuevas, F. Pauly, T. Huhn, E. Scheer, and A. Erbe, *Revealing the role of anchoring groups in the electrical conduction through single-molecule junctions*, Small **6**, 1529 (2010)
- [C3.6:26] \* ‡ A. Mishchenko, D. Vonlanthen, V. Meded, M. Bürkle, C. Li, I.V. Pobelov, A. Bagrets, J.K. Viljas, F. Pauly, F. Evers, M. Mayor, and T. Wandlowski, *Influence of conformation on conductance of biphenyl-dithiol single-molecule contacts*, Nano Lett. **10**, 156 (2010)
- [C3.6:27] \* ‡ A. Mishchenko, L.A. Zotti, D. Vonlanthen, M. Bürkle, F. Pauly, J.C. Cuevas, M. Mayor, and T. Wandlowski, *Single-Molecule Junctions Based on Nitrile-Terminated Biphenyls: A Promising New Anchoring Group*, J. Am. Chem. Soc. **133**, 184 (2011)
- [C3.6:28] Y. Kim, T.J. Hellmuth, M. Bürkle, F. Pauly, and E. Scheer, *Characteristics of amine-ended and thiol-ended alkane single-molecule junctions revealed by inelastic electron tunneling spectroscopy*, ACS Nano **5**, 4104 (2011)
- [C3.6:29] ‡ L.A. Zotti, M. Bürkle, Y.J. Dappe, F. Pauly, and J.C. Cuevas, *Electronic transport through single noble gas atoms*, Phys. Rev. B **84**, 193404 (2011)
- [C3.6:30] \* ‡ M. Bürkle, J. K. Viljas, A. Mishchenko, D. Vonlanthen, G. Schön, M. Mayor, T. Wandlowski, and F. Pauly, *Conduction mechanisms in biphenyl-dithiol single-molecule junctions*, arXiv:1109.0273 [cond-mat.mes-hall]

### C3.8 ‘Self-Assembled Molecules as Pre-Organized Building Blocks of Nanoscale Networks and Structures’ (M. Mayor)

- [C3.8:1] L. Shu, Z. Mu, H. Fuchs, L. Chi, and M. Mayor, *A self assembled molecular zipper based on a perfluorophenyl-phenyl diacetylene motif*, Chem. Comm. 1862 (2006)
- [C3.8:2] L. Shu and M. Mayor, *Shape persistent macrocycle with a self complementary recognition pattern based on diacetylene linked alternating hexylbenzene- and perfluorobenzene- rings*, Chem. Comm. 4134 (2006)
- [C3.8:3] Z. Mu, L. Shu, H. Fuchs, M. Mayor, and L. Chi, *Two Dimensional Chiral Networks Emerging from the Aryl-F···H Hydrogen-Bond-Driven Self-Assembly of Partially Fluorinated Rigid Molecular Structures*, J. Am. Chem. Soc. **130**, 10840 (2008)
- [C3.8:4] \* ‡ L. Shu, M. Müri, R. Krupke, M. Mayor, *Shape-persistent macrocycles comprising perfluorinated benzene subunits: synthesis, aggregation behaviour and unexpected  $\mu$ -rod formation*, Org. Biomol. Chem. **7**, 1081 (2009)
- [C3.8:5] \* ‡ C. Pérez León, C. Sürgers, M. Mayor, M. Marz, R. Hoffmann, and H. v. Löhneysen, *STM Investigation of Large  $\pi$ -Conjugated Oligomers and Tetrahydrofuran Codeposited on Cu(111) by Pulse Injection*, J. Phys. Chem. C, **113**, 14335 (2009)
- [C3.8:6] \* ‡ M. Barczewski, S. Walheim, T. Heiler, A. Błaszczyk, M. Mayor, T. Schimmel, *High Aspect Ratio Constructive Nanolithography with a Photo Dimerizable Molecule*, Langmuir **26**, 3623 (2010)
- [C3.8:7] ‡ A. Dreas-Włodarczak, M. Müllneritsch, T. Juffmann, C. Cioffi, M. Arndt, and M. Mayor, *Immobilization of Zinc Porphyrin Complexes on Pyridine-Functionalized Glass Surfaces*, Langmuir **26**, 10822 (2010)
- [C3.8:8] \* ‡ C.W. Marquardt, S. Grunder, A. Błaszczyk, S. Dehm, F. Hennrich, H. v. Löhneysen, M. Mayor, and R. Krupke, *Electroluminescence from a single nanotube-molecule-nanotube junction*, Nature Nanotechnology **5**, 863 (2010)
- [C3.8:9] \* ‡ F.A. Lemasson, T. Strunk, P. Gerstel, F. Hennrich, S. Lebedkin, C. Barner-Kowollik, W. Wenzel, M.M. Kappes, and M. Mayor, *Selective Dispersion of Single- Walled Carbon Nanotubes with Specific Chiral Indices by Poly(N-decyl-2,7-carbazole)*, J. Am. Chem. Soc. **133**, 652 (2011)
- [C3.8:10] \* ‡ S. Grunder, D. Muñoz Torres, C. Marquardt, A. Błaszczyk, R. Krupke, and M. Mayor, *Synthesis and Optical Properties of Molecular Rods Comprising a Central Core-Substituted Naphthalenediimide Chromophore for Carbon Nanotube Junctions*, Eur. J. Org. Chem. 478 (2011)
- [C3.8:11] ‡ Z. Mu, L. Shu, H. Fuchs, M. Mayor, and L. Chi, *Two-dimensional Self-Assembly of Linear Molecular Rods at Liquid/Solid Interface*, Langmuir **27**, 1359 (2011)
- [C3.8:12] \* N. Berton, F. Lemasson, J. Tittmann, N. Stürzl, F. Hennrich, M. Kappes, and M. Mayor, *Copolymer-controlled diameter-selective dispersion of semiconducting single-walled carbon nanotubes*, Chem. Mater. **23**, 2237 (2011)
- [C3.8:13] ‡ S. Eibenberger, S. Gerlich, M. Arndt, J. Tüxen, and M. Mayor, *Electric moments in molecule interferometry*, New J. Phys. **13**, 043033 (2011)
- [C3.8:14] \* F. Lemasson, J. Tittmann, F. Hennrich, N. Stürzl, S. Malik, M.M. Kappes, and M. Mayor, *Debundling, selection and release of SWNTs using fluorene-based photocleavable polymers*, Chem. Commun. **47**, 7428 (2011)

### C3.11 ‘Theoretical Spectroscopy of Molecular Nanostructures’ (F. Evers)

- [C3.11:1] ‡ M.J. van Setten, R. Gremaud, G. Brocks, B. Dam, G. Kresse, and G.A. de Wijs, *Optical response of the sodium alanate system: GW<sub>0</sub>-BSE calculations and thin film measurements*, Phys. Rev. B **83**, 035422 (2011)
- [C3.11:2] ‡ M. Gonzalez-Silveira, R. Gremaud, H. Schreuders, M.J. van Setten, E. Batyrev, A. Rougier, L. Dupont, E.G. Bardaji, W. Lohstroh, and B. Dam, *In-situ Deposition of Alkali and Alkaline Earth Hydride Thin Films to Investigate the Formation of Reactive Hydride Composites*, J. Phys. Chem. C **114**, 13895 (2010)
- [C3.11:3] V. Meded, A. Arnold, A. Bagrets, and F. Evers, *Molecular Switch Controlled by Pulsed Bias Voltages*, Small **5**, 2218 (2009)
- [C3.11:4] \* ‡ V. Meded, A. Bagrets, K. Fink, R. Chandrasekhar, M. Ruben, F. Evers, A. Bernand-Mantel, J.S. Seldenthuis, A. Beukman, and H.S.J. van der Zant, *Electrical control over the Fe(II) spin crossover in a single molecule: Theory and Experiment*, Phys. Rev. B **83**, 245415 (2011)
- [C3.11:5] \* A. Bagrets, R. Werner, F. Evers, G. Schneider, D. Schooss, and P. Wölfle, *Lowering of surface melting temperature in atomic clusters with a nearly closed shell structure*, Phys. Rev. B **81**, 075435 (2010)
- [C3.11:6] F. Evers, and P. Schmitteckert, *Broadening of the derivative discontinuity in density functional theory*, Phys. Chem. Chem. Phys. **13**, 14417 (2011)
- [C3.11:7] E.G. Bardaji, Z. Zhao-Karger, N. Boucharat, A. Nale, M.J. van Setten, W. Lohstroh, E. Röhm, M. Catti, and M. Fichtner, *LiBH<sub>4</sub>-Mg(BH<sub>4</sub>)<sub>2</sub>: A Physical Mixture of Metal Borohydrides as Hydrogen Storage Material*, J. Phys. Chem. **115**, 6095 (2011)
- [C3.11:8] F. Gebert, B. Willenberg, M.J. van Setten, E.G. Bardaji, E. Röhm, M. Fichtner, and J. Schoenes, *Polarization-dependent Raman spectroscopy of LiBH<sub>4</sub>- single crystals and Mg(BH<sub>4</sub>)<sub>2</sub> powders*, J. Raman Spectroscopy **42**, 1796 (2011)

### C3.12 ‘Nanoscale Luminescent Materials for Blue Light Excitation’ (C. Feldmann)

- [C3.12:1] G. Bübler, A. Zharkouskaya, and C. Feldmann, *Ionic Liquid based Approach to Nanoscale Functional Materials*, Solid State Sci. **10**, 461 (2008)
- [C3.12:2] \* A. Zharkouskaya, C. Feldmann, K. Trampert, W. Heering, and U. Lemmer, *Ionic Liquid based Approach to Luminescent LaPO<sub>4</sub>:Ce,Tb Nanocrystals: Synthesis, Characterization and Application*, Eur. J. Inorg. Chem. 873 (2008)
- [C3.12:3] M. Roming and C. Feldmann, *Selective Synthesis of α- and β-SrHPO<sub>4</sub> Nanoparticles*, J. Mater. Sci. **43**, 5504 (2008)
- [C3.12:4] M. Roming and C. Feldmann, *Anorganisch-organischer Kompositeuchtstoff*, Patent application, DE 102008009541.9, WO 2009/100800 A1
- [C3.12:5] M. Roming, C. Feldmann, Y.S. Avadhut, and J. Schmedt auf der Günne, *Characterization of Noncrystalline Nanomaterials: NMR of Zinc Phosphate as a Case Study*, Chem. Mater. **20**, 5787 (2008)
- [C3.12:6] M. Roming and C. Feldmann, *Synthesis and Characterization of Nanoscaled BiPO<sub>4</sub> and BiPO<sub>4</sub>:Tb*, J. Mater. Sci. **44**, 1412 (2009)
- [C3.12:7] M. Mai and C. Feldmann, *Two-color Emission of Zn<sub>2</sub>SiO<sub>4</sub>:Mn from Ionic Liquid mediated Synthesis*, Solid State Sci. **11**, 528 (2009)
- [C3.12:8] ‡ V. Pankratov, A.I. Popov, S.A. Chernov, A. Zharkouskaya, and C. Feldmann, *Mechanism for energy transfer processes between Ce<sup>3+</sup> and Tb<sup>3+</sup> in LaPO<sub>4</sub>:Ce,Tb nanocrystals by time-resolved luminescence spectroscopy*, phys. stat. sol. (b) **247**, 2252 (2010)
- [C3.12:9] A. Zharkouskaya, H. Lünsdorf, and C. Feldmann, *Ionic Liquid-Based Synthesis of Luminescent YVO<sub>4</sub>:Eu and YVO<sub>4</sub>:Eu@YF<sub>3</sub> Nanocrystals*, J. Mater. Sci. **44**, 3936 (2009)
- [C3.12:10] C.J. Höller, M. Mai, C. Feldmann, and K. Müller-Buschbaum, *The Interaction of Rare Earth Chlorides with 4,4'-Bipyridine for the Reversible Formation of Template Based Luminescent Ln-N-MOFs*, Dalton Trans. **39**, 461 (2010)
- [C3.12:11] M. Roming, H. Lünsdorf, K.E.J. Dittmar, and C. Feldmann, *ZrO(HPO<sub>4</sub>)<sub>1-x</sub>(FMN)<sub>x</sub>: Quick and Easy Synthesis of a Nanoscale Luminescent Biomarker*, Angew. Chem. Int. Ed. **49**, 632 (2010)
- [C3.12:12] S. Becht, S. Ernst, H. Bappert, and C. Feldmann, *Do-it-yourself! Nanomaterialien zum Anfassen*, Chem. Unserer Zeit **44**, 14 (2010)
- [C3.12:13] M. Roming and C. Feldmann, *Zirconium Umbelliferonephosphate – A Luminescent Organic-Inorganic Hybrid Nanomaterial*, Solid State Sci. **13**, 508 (2011)
- [C3.12:14] A. Zurawski, M. Mai, D. Baumann, C. Feldmann, and K. Müller-Buschbaum, *Homoleptic Imidazolate Frameworks <sup>3</sup>[Sr<sub>1-x</sub>Eu<sub>x</sub>(Im)<sub>2</sub>] – Hybrid Materials with Efficient and Tuneable Luminescence*, Chem. Commun. **47**, 496 (2011)
- [C3.12:15] ‡ V. Pankratov, A.I. Popov, A. Kotlov, and C. Feldmann, *Luminescence of nano- and macrosized LaPO<sub>4</sub>:Ce,Tb excited by synchrotron sadiation*, Opt. Mater. **33**, 1102 (2011)
- [C3.12:16] P. Schmitt, N. Brem, S. Schunk, and C. Feldmann, *Polyol-Mediated Synthesis and Properties of Nanoscale Molybdates/Tungstates: Color, Luminescence, Catalysis*, Adv. Funct. Mater. **21**, 3037 (2011)
- [C3.12:17] C. Feldmann, *Luminescent Nanomaterials*, Nanoscale **3**, 1947 (2011)

- [C3.12:18] \* V. Pankratov, A.I. Popov, L. Shirmane, A. Kotlov, and C. Feldmann, *LaPO<sub>4</sub>:Ce,Tb and YVO<sub>4</sub>:Eu Nanophosphors: Luminescence Studies in the Vacuum-ultraviolet Spectral Range*, J. Appl. Phys. **110**, 053522 (2011)
- [C3.12:19] M. Mai and C. Feldmann, *Microemulsion-based Synthesis and Luminescence of Nanoparticulate CaWO<sub>4</sub>, ZnWO<sub>4</sub>, CaWO<sub>4</sub>:Tb and CaWO<sub>4</sub>:Eu*, J. Mater. Sci., DOI 10.1007/s10853-011-5923-8 (2012)

### C3.13 ‘Subsystem Quantum Chemistry for Nanostructures’ (Ch. Jacob)

- [C3.13:1] ‡ S. Fux, Ch. R. Jacob, J. Neugebauer, L. Visscher, and M. Reiher, *Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds*, *J. Chem. Phys.* **132**, 164101 (2010)
- [C3.13:2] ‡ V. Liégeois, Ch.R. Jacob, B. Champagne, and M. Reiher, *Analysis of vibrational Raman optical activity signatures of the  $(TG)_N$  and  $(GG)_N$  conformations of isotactic polypropylene chains in terms of localized modes*, *J. Phys. Chem. A* **114**, 7198 (2010)
- [C3.13:3] ‡ T. Weymuth, Ch.R. Jacob, and M. Reiher, *A local mode model for understanding the dependence of the extended amide III vibrations on secondary structure*, *J. Phys. Chem. B* **114**, 10649 (2010)
- [C3.13:4] ‡ T. Weymuth, Ch.R. Jacob, and M. Reiher, *Identifying protein  $\beta$ -turns with vibrational Raman optical activity*, *ChemPhysChem* **12**, 1165 (2011)
- [C3.13:5] ‡ Ch.R. Jacob, S.M. Beyhan, R.E. Bulo, A.S.P. Gomes, A.W. Götz, K. Kiewisch, J. Sikkema, and L. Visscher, *PyADF – A scripting framework for multiscale quantum chemistry*, *J. Comput. Chem.* **32**, 2328 (2011)
- [C3.13:6] ‡ N.S. Bieler, M.P. Haag, Ch.R. Jacob, and M. Reiher, *Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides*, *J. Chem. Theory Comput.* **12**, 1867 (2011)
- [C3.13:7] ‡ S. Fux, Ch.R. Jacob, J. Neugebauer, L. Visscher, and M. Reiher, *Response to Comment on ‘Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds’*, *J. Chem. Phys.* **135**, 027102 (2011)
- [C3.13:8] ‡ K. Boguslawski, Ch.R. Jacob, and M. Reiher, *Can DFT accurately predict spin densities? Analysis of discrepancies in iron nitrosyl complexes*, *J. Chem. Theory Comput.* **7**, 2740 (2011)
- [C3.13:9] Ch.R. Jacob, *Theoretical study of the Raman optical activity spectra of 310-helical polypeptides*, *ChemPhysChem* **12**, 3291 (2011)

## Project C4 ‘Molecular Nanostructures on Surfaces’

### C4.1 ,Site-Selective Coupling to Electrodes and Transport through Single Molecules (H. von Löhneysen / R. Krupke / M. Lukas)

- [C4.1:1] \* R. Krupke, S. Linden, M. Rapp, and F. Hennrich, *Thin films of metallic carbon nanotubes prepared by dielectrophoresis*, *Adv. Mater.* **18**, 1468 (2006)
- [C4.1:2] \* C.W. Marquardt, S. Blatt, F. Hennrich, H. v. Löhneysen, and R. Krupke, *Probing dielectrophoretic force fields with metallic carbon nanotubes*, *Appl. Phys. Lett.* **89**, 183117 (2006)
- [C4.1:3] \* F. Hennrich, R. Krupke, K. Arnold, J.A.R. Rojas Stütz, S. Lebedkin, T. Koch, T. Schimmel, and M.M. Kappes, *The Mechanism of Cavitation-Induced Scission of Single-Walled Carbon Nanotubes*, *J. Phys. Chem. B* **111**, 1932 (2007)
- [C4.1:4] \* A. Vijayaraghavan, S. Blatt, D. Weissenberger, M. Oron-Carl, F. Hennrich, D. Gerthsen, H. Hahn, and R. Krupke, *Ultra-Large-Scale Directed Assembly of Single-Walled Carbon Nanotube Devices*, *Nano Lett.* **7**, 1556 (2007)
- [C4.1:5] \* S. Blatt, F. Hennrich, H. v. Löhneysen, M.M. Kappes, A. Vijayaraghavan, and R. Krupke, *Influence of Structural and Dielectric Anisotropy on the Dielectrophoresis of Single-Walled Carbon Nanotubes*, *Nano Lett.* **7**, 1960 (2007)
- [C4.1:6] \* R. Krupke and F. Hennrich, Invited book chapter *Separation techniques for carbon nanotubes in Chemistry of carbon nanotubes*, Eds. V.A. Basiuk, and E.V. Basiuk (American Scientific Publishers, 2007) 129-139
- [C4.1:7] ‡ D.K. Aswal, S.P. Koiry, V. Saxena, N. Padma, S.K. Gupta, J.V. Yakhmi, S.K. Nayak, A. Singh, and C. Sürgers, *Electrografting of organic monolayers on silicon for molecular electronics* in Physics, Chemistry and Application of Nanostructures, edited by V.E. Borisenko, S.V. Gaponenko, and V.S. Gurin, (World Scientific, Singapore, 2007) p. 541
- [C4.1:8] \* C.W. Marquardt, S. Dehm, A. Vijayaraghavan, S. Blatt, F. Hennrich, and R. Krupke, *Reversible Metal–Insulator Transitions in Metallic Single-Walled Carbon Nanotubes*, *Nano Lett.* **9**, 2767 (2008)
- [C4.1:9] ‡ R.E.A. Kelly, M. Lukas, L.N. Kantorovich, R. Otero, W. Xu, M. Mura, E. Lægsgaard, I. Stensgaard, and F. Besenbacher, *Understanding the Disorder of the DNA Base Cytosine on the Au(111) Surface*, *J. Chem. Phys.* **129**, 184707 (2008)
- [C4.1:10] ‡ A.K. Chauhan, D.K. Aswal, S.P. Koiry, S.K. Gupta, J.V. Yakhmi, C. Sürgers, D. Guerin, S. Lenfant, and D. Vuillaume, *Self-assembly of the 3-aminopropyltrimethoxysilane multilayers on Si and hysteretic current-voltage characteristics*, *Appl. Phys. A* **90**, 581 (2008)
- [C4.1:11] ‡ A.K. Debnath, S. Samanta, A. Singh, D.K. Aswal, S.K. Gupta, J.V. Yakhmi, S.K. Deshpande, A.K. Poswal, and C. Sürgers, *Growth of iron phthalocyanine nanoweb and nanobrush using molecular beam epitaxy*, *Physica E* **41**, 154 (2008)
- [C4.1:12] \* C. Pérez León, C. Sürgers, M. Mayor, M. Marz, R. Hoffmann, H. v. Löhneysen, *STM investigation of large π-conjugated oligomers and tetrahydrofuran codeposited on Cu(111) by pulse injection*, *J. Phys. Chem. C* **113**, 14335 (2009)
- [C4.1:13] \* S. Dasgupta, M. Lukas, K. Dössel, R. Kruk, and H. Hahn, *Electron mobility variations in surface-charged indium tin oxide thin films*, *Phys. Rev. B* **80**, 085425 (2009)
- [C4.1:14] ‡ M. Lukas, R.E.A. Kelly, L.N. Kantorovich, R. Otero, W. Xu, M. Mura, E. Lægsgaard, I. Stensgaard and F. Besenbacher, *Adenine monolayers on the*

*Au(111) surface: Structure identification by scanning tunnelling microscopy experiment and ab initio calculations*, J. Chem. Phys. **130**, 024705 (2009)

- [C4.1:15] ‡ V. Saxena, A.K. Chauhan, N. Padma, D.K. Aswal, S.P. Koiry, S. Sen, R.B. Tokas, S.K. Gupta, C. Sürgers, and J.V. Yakhmi, *Poly(3-hexylthiopene) based field-effect transistors with gate SiO<sub>2</sub> dielectric modified by multi-layers of 3-aminopropyltrimethoxysilane*, Thin Solid Films **517**, 6124 (2009)
- [C4.1:16] \* C.W. Marquardt, S. Grunder, A. Błaszczyk, S. Dehm, F. Hennrich, H. v. Löhneysen, M. Mayor, and R. Krupke, *Electroluminescence from a single nanotube-molecule-nanotube junction*, Nature Nanotechnology **5**, 863 (2010)
- [C4.1:17] \* S. Grunder, D. Muñoz Torres, C.W. Marquardt, A. Błaszczyk, R. Krupke, and M. Mayor, *Synthesis and Optical Properties of Molecular Rods Comprising a Central Core-Substituted Naphthalenediimide Chromophore for Carbon Nanotube Junctions*, Eur. J. Org. Chem. 478 (2011)
- [C4.1:18] \* C. Thiele, M. Engel, F. Hennrich, M.M. Kappes, K.-P. Johnsen, C.G. Frase, H. v. Löhneysen, and R. Krupke, *Controlled fabrication of single-walled carbon nanotube electrodes by electron-beam-induced oxidation*, Appl. Phys. Lett. **99**, 173105 (2011)

#### C4.5 ‘Electron Microscopy Studies of Nanoparticles and Nanostructured Materials’ (D. Gerthsen)

- [C4.5:1] M. Wanner, D. Bach, D. Gerthsen, R. Werner, and B. Tesche, *Electron holography of thin amorphous carbon films: measurement of the mean inner potential and a thickness-independent phase shift*, Ultramicroscopy **106**, 341 (2006)
- [C4.5:2] M. Wanner, R. Werner, and D. Gerthsen, *Dynamics of gold clusters on amorphous carbon films induced by annealing in a transmission electron microscope*, Surf. Sci. **600**, 632 (2006)
- [C4.5:3] ‡ M. Schowalter, A. Rosenauer, D. Lamoen, P. Kruse, and D. Gerthsen, *Ab initio computation of the mean inner Coulomb potential of wurtzite-type semiconductors and gold*, Appl. Phys. Lett. **88**, 232108 (2006)
- [C4.5:4] \* C. Zimmermann, C. Feldmann, M. Wanner, and D. Gerthsen, *Nanoscale gold hollow spheres via microemulsion approach*, Small **3**, 1347 (2007)
- [C4.5:5] R. Popescu, E. Müller, D. Gerthsen, M. Wanner, M. Schowalter, and A. Rosenauer, *Mean inner potential and surface strain of Au clusters analysed by transmission electron holography*, Phys. Rev. B **76**, 235411 (2007)
- [C4.5:6] \* R. Popescu, R. Schneider, D. Gerthsen, M. Wanner, A. Böttcher, D. Löffler, P. Weiss, and M.M. Kappes, *Coarsening of mass-selected Au clusters on amorphous carbon at room temperature*, Surf. Sci. **603**, 3119 (2009)
- [C4.5:7] \* P. Leidinger, R. Popescu, D. Gerthsen, and C. Feldmann, *Nanoscale La(OH)<sub>3</sub> Hollow Spheres and Fine-Tuning of Its Outer Diameter and Cavity Size*, Small **6**, 1886 (2010)
- [C4.5:8] \* C. Kind, R. Popescu, E. Müller, D. Gerthsen, and C. Feldmann, *Microemulsion-based synthesis of nanoscaled silver hollow spheres and direct comparison with massive particles of similar size*, Nanoscale **2**, 2223 (2010)
- [C4.5:9] \* P. Leidinger, R. Popescu, D. Gerthsen, H. Lünsdorf, and C. Feldmann, *Nanoscale copper sulfide hollow spheres with phase-engineered composition: covellite (CuS), digenite (Cu<sub>1.8</sub>S), chalcocite (Cu<sub>2</sub>S)*, Nanoscale **3**, 2544 (2011)
- [C4.5:10] \* C. Zurmühl, R. Popescu, D. Gerthsen, and C. Feldmann, *Microemulsion-based synthesis of nanoscale TiO<sub>2</sub> hollow spheres*, Solid State Sciences **13**, 1505 (2011)
- [C4.5:11] \* Li Shang, A. Naghmeh, F. Stockmar, W. Send, V. Trouillet, M. Bruns, D. Gerthsen, and G.U. Nienhaus, *One-pot synthesis of near-infrared emitting, dihydroliopic acid capped gold clusters for cellular fluorescence imaging*, Small **7**, 2614 (2011)
- [C4.5:12] B. Gamm, H. Blank, R. Popescu, R. Schneider, A. Beyer, A. Götzhäuser, and D. Gerthsen, *Quantitative high-resolution transmission electron microscopy of single atoms*, Microsc. Microanal., DOI:10.1017/S1431927611012232

#### C4.6 ‘Support Interactions and Thermal Stability of Size-Selected Clusters Deposited onto Single-Crystal Surfaces’ (M. Kappes)

- [C4.6:1] D. Löffler, S. Jester, P. Weis, A. Böttcher, and M.M. Kappes, *C<sub>n</sub> Films (n=50, 52, 54, 56 and 58) on Graphite: Cage Size Dependent Electronic Properties*, *J. Chem. Phys.* **124**, 054705 (2006)
- [C4.6:2] S. Jester, P. Weis, M. Hillenkamp, O. Ehrler, A. Böttcher, and M. Kappes, *Quantifying electron transfer during hyperthermal scattering of C<sub>60</sub><sup>+</sup> from Au(111) and n-alkylthiol self-assembled monolayers*, *J. Chem. Phys.* **124**, 144704 (2006)
- [C4.6:3] \* R. Ahlrichs, N.R.M. Crawford, A. Eichhöfer, D. Fenske, O. Hampe, M.M. Kappes, and J. Olkowska-Oetzel, *Synthesis and Structure of Two Ionic Copper-Indium-Selenolate Cluster Complexes (As(C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>)<sub>2</sub>[Cu<sub>6</sub>In<sub>4</sub>(SeC<sub>6</sub>H<sub>5</sub>)<sub>16</sub>Cl<sub>4</sub>] and (As(C<sub>6</sub>H<sub>5</sub>)<sub>4</sub>)<sub>2</sub>[Cu<sub>7</sub>In<sub>4</sub>(SeC<sub>6</sub>H<sub>5</sub>)<sub>20</sub>]*, *Eur. J. Inorg. Chem.* 345 (2006)
- [C4.6:4] \* P. Sevillano, O. Fuhr, M. Kattanek, P. Nava, O. Hampe, S. Lebedkin, R. Ahlrichs, D. Fenske and M.M. Kappes, *The Phosphine-Stabilized Gold–Arsenic Cluster compounds [Au<sub>19</sub>(AsnPr)<sub>8</sub>(dppe)<sub>6</sub>]Cl<sub>3</sub>, [Au<sub>10</sub>(AsnPr)<sub>4</sub>]<sub>2</sub>(dppe)<sub>4</sub>]Cl<sub>2</sub>, [Au<sub>17</sub>(AsnPr)<sub>6</sub>(As<sub>2</sub>nPr)(dppm)<sub>6</sub>]Cl<sub>3</sub> and [Au<sub>10</sub>(AsPh)<sub>4</sub>(dppe)<sub>4</sub>]Cl<sub>2</sub>. Synthesis, Characterization, and DFT Calculations*, *Angew. Chem. Int. Ed.* **45**, 3702 (2006)
- [C4.6:5] M. Blom, D. Schooss, J. Stairs and M.M. Kappes, *Experimental Structure Determination of Silver Cluster Ions (Ag<sub>n</sub><sup>+</sup>, 19 ≤ n ≤ 79)*, *J. Chem. Phys.* **124**, 244308 (2006)
- [C4.6:6] \* M. Neumaier, F. Weigend, O. Hampe and M.M. Kappes, *Reactions of mixed silver-gold cluster cations Ag<sub>m</sub>Au<sub>n</sub><sup>+</sup> (m+n=4,5,6) with CO: Radiative association kinetics and DFT computations*, *J. Chem. Phys.* **125**, 104308 (2006)
- [C4.6:7] D. Löffler, S.-S. Jester, P. Weis, A. Böttcher and M.M. Kappes, *Deuteration-induced Scission of C<sub>58</sub> Oligomers*, *J. Chem. Phys.* **125**, 224705 (2006)
- [C4.6:8] \* A. Böttcher, M. Heil, N. Stürzl, S.S. Jester, S. Malik, F. Perez-Willard, P. Brenner, D Gerthsen, M.M. Kappes, *Nanostructuring the graphite basal plane by focused-ion-beam patterning and oxygen etching*, *Nanotechnol.* **17**, 5889 (2006)
- [C4.6:9] ‡ A. Lechtken, D. Schooss, J.R. Stairs, M.M. Blom, F. Furche, B. von Issendorff, and M.M. Kappes, *Au<sub>34</sub><sup>-</sup>: A Chiral Gold Cluster?*, *Angew. Chem. Int. Ed.* **46**, 2944 (2007)
- [C4.6:10] \* P. Sevillano, O. Fuhr, O. Hampe, S. Lebedkin, E. Matern, D. Fenske, and M.M. Kappes, *Synthesis, Characterization and X-Ray Structure Determination of [Au<sub>18</sub>(P)<sub>2</sub>(PPh)<sub>4</sub>(PPhH)(dppm)<sub>6</sub>]Cl<sub>3</sub>*, *Inorg. Chem.* **46**, 7294 (2007)
- [C4.6:11] D. Loeffler, P. Weis, A. Boettcher, and M. Kappes, *Thermal stability of deuterated C<sub>60</sub> films*, *J. Phys. Chem. C* **111**, 17743 (2007)
- [C4.6:12] \* P. Sevillano, O. Fuhr, O. Hampe, S. Lebedkin, C. Weiss, R. Ahlrichs, D. Fenske, and M.M. Kappes, *Synthesis, Characterization, and quantum mechanical calculations of [Au<sub>18</sub>Se<sub>8</sub>(Dppphph<sub>6</sub>)<sub>2</sub>]Cl<sub>2</sub>*, *Eur. J. Inorg. Chem.* **33**, 5163 (2007)
- [C4.6:13] \* E. Oger, N.R.M. Crawford, R. Kelting, P. Weis, M.M. Kappes, and R. Ahlrichs, *Boron cluster cations: transition from planar to cylindrical structures*, *Angew. Chem. Int. Ed.* **46**, 8503 (2007)
- [C4.6:14] ‡ J.B. Tracy, M.C. Crowe, J.F. Parker, O. Hampe, C.A. Fields-Zinna, A. Dass, and R.W. Murray, *Electrospray Ionization Mass Spectrometry of Uniform and Mixed Monolayer Nanoparticles: Au<sub>25</sub>[S(CH<sub>2</sub>)<sub>2</sub>Ph]<sub>18</sub> and Au<sub>25</sub>[S(CH<sub>2</sub>)<sub>2</sub>Ph]<sub>18-x</sub>(SR)<sub>x</sub>*, *J. Am. Chem. Soc.* **129**, 16209 (2007)

- [C4.6:15] \* A. Eichhöfer and O. Hampe, *Investigating the thermolysis products of  $[Cd_{10}Se_4(SePh)_{12}(PnPr_3)_4]$  – the new cluster ion  $[Cd_{17}Se_4(SePh)_{28}]^{2-}$* , J. Cluster Sci. **18**, 494 (2007)
- [C4.6:16] \* R. Popescu, E. Müller, M. Wanner, D. Gerthsen, M. Schowalter, A. Rosenauer, A. Böttcher, D. Löffler, and P. Weis, *Increase of the mean inner Coulomb potential in Au clusters induced by surface tension and its implication for electron scattering*, Phys. Rev. B **76**, 235411 (2007)
- [C4.6:17] D. Loeffler, P. Weis, S. Malik, A. Böttcher, and M. Kappes, *Thermal Stability, Phase Segregation and Sublimation of Cesium Fulleride Thin Films*, Phys. Rev. B **77**, 155405 (2008)
- [C4.6:18] ‡ M.P. Johansson, F. Furche, A. Lechtken, D. Schooss, and M.M. Kappes, *2D-3D transition of gold cluster anions resolved*, Phys. Rev. A **77**, 053202 (2008)
- [C4.6:19] A.N. Gloess, H. Schneider, J.M. Weber, and M.M. Kappes, *Electronically excited states and visible region photodissociation spectroscopy of  $Au_m^+ \cdot Ar_n$  clusters ( $m=7-9$ ): molecular dimensionality transition?*, J. Chem. Phys. **128**, 114312 (2008)
- [C4.6:20] D. Löffler, P. Weis, A. Böttcher, and M.M. Kappes, *Thermally triggered dedeuteriation of cesium-doped deuterofullerene films*, J. Phys. Chem. C **112**, 13789 (2008)
- [C4.6:21] \* M. Neumaier, F. Weigand, O. Hampe, and M.M. Kappes, *Binding energy and preferred adsorption sites of CO on gold and silver-gold cluster cations: Adsorption kinetics and quantum chemical calculations*, Faraday Discuss. **138**, 393 (2008)
- [C4.6:22] \* A. Lechtken, C. Neiss, J. Stairs, and D. Schooss, *Comparative study of the structures of copper, silver and gold icosamers – influence of metal type and charge state*, J. Chem. Phys. **129**, 154304 (2008)
- [C4.6:23] \* R. Popescu, R. Schneider, D. Gerthsen, A. Böttcher, D. Löffler, P. Weis, and M.M. Kappes, *Coarsening of mass-selected Au clusters on amorphous carbon at room temperature*, Surf. Sci. **603**, 3119 (2009)
- [C4.6:24] \* A. Lechtken, C. Neiss, M.M. Kappes, and D. Schooss, *Structure Determination of Gold Clusters by Trapped Ion Electron Diffraction:  $Au_{14}^- - Au_{19}^-$* , Phys. Chem. Chem. Phys. **11**, 4344 (2009)
- [C4.6:25] \* E. Oger, R. Kelting, P. Weis, A. Lechtken, D. Schooss, N.R.M. Crawford, R. Ahlrichs, and M.M. Kappes, *Small tin cluster anions - Transition from quasi-spherical to prolate structures*, J. Chem. Phys. **130**, 124305 (2009)
- [C4.6:26] ‡ L.-M. Wang, J. Bai, A. Lechtken, W. Huang, D. Schooss, M.M. Kappes, X.C. Zeng, and L.-S. Wang, *Magnetic Doping of the Golden Cage Cluster:  $M@Au_{16}^-$  ( $M=Fe, Co, Ni$ )*, Phys. Rev. B **79**, 033413 (2009)
- [C4.6:27] ‡ \* D. Löffler, N. Bajales, M. Cudaj, P. Weis, S. Lebedkin, A. Bihlmeier, D.P. Tew, W. Klopper, A. Böttcher, and M.M. Kappes, *Non-IPR  $C_{60}$  Solids*, J. Chem. Phys. **130**, 164705 (2009)
- [C4.6:28] \* A. Lechtken, N. Drebov, R. Ahlrichs, M.M. Kappes, and D. Schooss, *Communications: Tin Cluster Anions ( $Sn_n^-$ ,  $n=18, 20, 23$ , and 25) Comprise Dimers of Stable Subunits*, J. Chem. Phys. **132**, 211102 (2010)
- [C4.6:29] D. Schooss, P. Weis, O. Hampe, and M.M. Kappes, *Determining the Size-Dependent Structure of Ligand-free Gold-Cluster Ions*, Phil. Trans. R. Soc. A **368**, 1211 (2010)

- [C4.6:30] D. Löffler, S. Ulas, S.-S. Jester, P. Weis, A. Böttcher, and M.M. Kappes, *Properties of non-IPR fullerene films versus size of the building blocks*, Phys. Chem. Chem. Phys. **12**, 10671 (2010)
- [C4.6:31] \* N. Drebov, E. Oger, T. Rapps, R. Kelting, D. Schooss, P. Weis, M. Kappes, and R. Ahlrichs, *Structure of Tin Cluster Cations  $Sn_3^+$  to  $Sn_{15}^+$* , J. Chem. Phys. **133**, 224302 (2010)
- [C4.6:32] \* R. Kelting, R. Otterstätter, P. Weis, N. Drebov, R. Ahlrichs, and M.M. Kappes, *Structures and Energetics of Small Lead Cluster Ions*, J. Chem. Phys. **134**, 024311 (2011)
- [C4.6:33] S.S. Jester, D. Löffler, P. Weis, A. Böttcher, and M.M. Kappes, *Morphology of  $C_n$  thin films ( $50 \leq n < 60$ ) on graphite: Inference of energy dissipation during hyperthermal deposition*, Surf. Sci. **603**, 1863 (2009)
- [C4.6:34] ‡ \* J. Fang, S. Du, S. Lebedkin, Z. Li, R. Kruk, M. Kappes, and H. Hahn, *Gold Mesostructures with Tailored Surface Topography and Their Self-Assembly Arrays for Surface-Enhanced Raman Spectroscopy*, Nano Lett. **10**, 5006 (2010)
- [C4.6:35] \* A. Wiesel, N. Drebov, T. Rapps, R. Ahlrichs, U. Schwarz, R. Kelting, P. Weis, M. Kappes, and D. Schooss, *Structures of medium sized tin cluster anions*, Phys. Chem. Chem. Phys. **14**, 234 (2012)

#### C4.8 ‘Fabrication and Optical Characterization of Metal Nanostructures’ (R. Schuster)

- [C4.8:1] R. Schuster, *Electrochemical Microstructuring with Short Voltage Pulses*, ChemPhysChem **8**, 34 (2007)
- [C4.8:2] X. Ma, A. Bán, and R. Schuster, *Electrochemical Machining of Gold Microstructures in LiCl/Dimethyl Sulfoxide*, ChemPhysChem **11**, 616 (2010)
- [C4.8:3] X. Ma and R. Schuster, *Locally Enhanced Cathodoluminescence of Electrochemically Fabricated Gold Nanostructures*, J. Electroanal. Chem. **662**, 12 (2011)

**C4.9 ‘Electrochemistry with an Electron Beam – Local Metal Deposition in Ionic Liquids and Molten-Salt Thin Films (R. Schuster)**

[C4.9:1] V. Halka, M.J. Schmid, V. Avrutskiy, X. Ma, and R. Schuster, *Electron-Beam-Induced Deposition of Metallic Microstructures from a Molten-Salt Film on Conductive and Nonconductive Substrates*, Angew. Chem. Int. Ed. **50**, 4692 (2011)

**C4.11 ‘Theory and Simulation of Molecular Materials and Functionality’ (P. Wölfle / F. Evers)**

- [C4.11:1] \* S. Bera, A. Arnold, F. Evers, R. Narayanan, and P. Wölfle, *Elastic properties of graphene flakes: Boundary effects and lattice vibrations*, Phys. Rev. B **82**, 195445 (2010)
- [C4.11:2] \* P.M. Ostrovsky, M. Titov, S. Bera, I.V. Gornyi, and A.D. Mirlin, *Diffusion and criticality in undoped graphene with resonant scatterers*, Phys. Rev. Lett. **105**, 266803 (2010)
- [C4.11:3] \* I.S. Burmistrov, S. Bera, F. Evers, I.V. Gornyi, and A.D. Mirlin, *Wavefunction Multifractality and dephasing at metal-insulator and quantum Hall transitions*, Ann. Phys. **326**, 1457 (2011)
- [C4.11:4] \* A. Mischchenko, D. Vonlanthen, M. Bürkle, J. Vilas, F. Pauly, V. Meded, A. Bagrets, C. Li, I. Pobelov, F. Evers, M. Mayor, and T. Wandlowski, *Influence of Conformation on the Conductance of Biphenyl-Dithiol Single-Molecule Contacts*, Nano Lett. **10**, 156 (2010)
- [C4.11:5] \* M. Bürkle, J.K. Viljas, A. Mishchenko, D. Vonlanthen, G. Schoen, M. Mayor, T. Wandlowski, and F. Pauly, *Conduction mechanisms in biphenyl-dithiol single-molecule junctions*, arXiv:1109.0273v1
- [C4.11:6] \* S. Schmaus, A. Bagrets, Y. Nahas, T.K. Yamada, A. Bork, M. Bowen, E. Beaurepaire, F. Evers, and W. Wulfhekel, *Giant magnetoresistance through a single molecule*, Nature Nanotechnology **6**, 185 (2011)
- [C4.11:7] M. Polok, D.V. Fedorov, A. Bagrets, P. Zahn, and I. Mertig, *Evaluation of conduction eigenchannels of an adatom probed by an STM tip*, Phys. Rev. B **83**, 245426 (2011)