

Publication list of Dr. Alexey A. Popov (as of 24.02.2011)

Reviews and book chapters

1. A. A. Popov. "Metal-Cage Bonding, Molecular Structures and Vibrational Spectra of Endohedral Fullerenes: Bridging Experiment and Theory". *J. Comput. Theor. Nanosci.* **2009**, 6 (2), 292-317.
2. O. V. Boltalina, A. A. Popov, S. H. Strauss, "Physicochemical Properties and the Unusual Structure of Fullerenes: Single-crystal X-ray Structures of Fullerenes and Their Derivatives" in *Strained Hydrocarbons: Beyond the van't Hoff and Le Bel Hypothesis*, H. Dodzik (Editor), Wiley-VCH, Weinheim, **2009**, pp. 225-238.
3. A. A. Popov, "Physicochemical Properties and the Unusual Structure of Fullerenes: Vibrational and Electronic Spectra" in *Strained Hydrocarbons: Beyond the van't Hoff and Le Bel Hypothesis*, H. Dodzik (Editor), Wiley-VCH, Weinheim, **2009**, pp. 238-249.

Full papers in scientific journals

1998-2003

1. P. A. Dorozhko, A. A. Popov, M. V. Korobov, B. L. Tumanskii. "Stability of Gaseous Fullerene Chlorides". *Chem. Phys. Lett.* **1998**, 287, 154-161. DOI: [10.1016/S0009-2614\(98\)00136-5](https://doi.org/10.1016/S0009-2614(98)00136-5)
2. R. G. Gasanov, O. G. Kalina, A. A. Popov, P. A. Dorozhko, B. L. Tumanskii. "ESR Study of the photolysis of C₆₀Cl₆," *Russ. Chem. Bull.* **2000**, 4, 753-753. (P. Г. Гасанов, О. Г. Калина, А. А. Попов, П. А. Дорожко, Б. Л. Туманский "Исследование методом ЭПР фотолиза C₆₀Cl₆". *Изв. Акад. Наук., Сер. Хим.* **2000**, 4, 752-753). DOI: [10.1007/BF02495497](https://doi.org/10.1007/BF02495497)
3. P. A. Dorozhko, A. S. Lobach, A. A. Popov, V. M. Senyavin, M. V. Korobov. "Sublimation of Hydrofullerenes C₆₀H₃₆ and C₆₀H₁₈," *Chem. Phys. Lett.* **2001**, 336, 39-46. DOI: [10.1016/S0009-2614\(01\)00103-8](https://doi.org/10.1016/S0009-2614(01)00103-8)
4. P. A. Troshin, D. Kolesnikov, A. V. Burtsev, R. N. Lubovskaya, N. I. Denisenko, A. A. Popov, S. I. Troyanov, O. V. Boltalina. "Bromination of [60]Fullerene. I. High-Yield Synthesis of C₆₀Br_x (x = 6, 8, 24)," *Fullerenes Nanotubes Carbon Nanostr.* **2003**, 11, 47-60. DOI: [10.1081/FST-120018666](https://doi.org/10.1081/FST-120018666)
5. S. I. Troyanov, A. A. Popov, N. I. Denisenko, O. V. Boltalina, L. N. Sidorov, E. Kemnitz. "The First X-ray Crystal Structures of Halogenated [70]Fullerene: C₇₀Br₁₀ and C₇₀Br₁₀·3Br₂," *Angew. Chem. Int. Ed.* **2003**, 42, 2395-2398. DOI: [10.1002/anie.200351132](https://doi.org/10.1002/anie.200351132)

2004

6. J. V. Rau, S. Nunziante Cesaro, O. V. Boltalina, V. Agafonov, A. A. Popov, L. N. Sidorov. "Raman and Infrared Spectroscopic Study of C₆₀F₁₈, C₆₀F₃₆ and C₆₀F₄₈," *Vibrational Spectroscopy* **2004**, 34, 137-147. DOI: [10.1016/j.vibspec.2003.05.003](https://doi.org/10.1016/j.vibspec.2003.05.003)
7. A. A. Popov, V. M. Senyavin, A. A. Granovsky. "Vibrations of Bromofullerene C₆₀Br₂₄: C₆₀ Cage Confined Into Static Bromine Sphere," *Chem. Phys. Lett.* **2004**, 383, 149-155. DOI: [10.1016/j.cplett.2003.10.144](https://doi.org/10.1016/j.cplett.2003.10.144)
8. V. I. Korepanov, A. A. Popov, V. M. Senyavin, M. Reinov, M. A. Yurovskaya, "Infrared Spectra and Structure of C₆₀ Heterocyclic Derivatives," *Fullerenes Nanotubes Carbon Nanostr.* **2004**, 12, 209-213. DOI: [10.1081/FST-120027158](https://doi.org/10.1081/FST-120027158)
9. V. M. Senyavin, A. A. Popov, A. A. Granovsky, V. A. Davydov, V. N. Agafonov, "Ab initio and DFT-Based Assignment of the Vibrational Spectra of Polymerized Fullerenes," *Fullerenes Nanotubes Carbon Nanostr.* **2004**, 12, 253-258. DOI: [10.1081/FST-120027165](https://doi.org/10.1081/FST-120027165)

10. A. A. Popov, V. M. Senyavin, A. A. Granovsky. "Vibrational Spectra of Chloro- and Bromofullerenes," *Fullerenes Nanotubes Carbon Nanostr.* **2004**, *12*, 305-310. DOI: [10.1081/FST-120027184](https://doi.org/10.1081/FST-120027184)
11. N. I. Denisenko, S. I. Troyanov, A. A. Popov, I. V. Kuvychko, B. Zemva, E. Kemnitz, S. H. Strauss, O. V. Boltalina. " T_h -C₆₀F₂₄", *J. Am. Chem. Soc.* **2004**, *126*, 1618-1619. DOI: [10.1021/ja039361f](https://doi.org/10.1021/ja039361f)
12. S. I. Troyanov, N. B. Shustova, A. A. Popov, M. Feist, E. Kemnitz. "Chlorination of C₆₀ and C₇₀ Fullerenes Using SbCl₅ and VCl₄ Chlorides". *Russ. J. Inorg. Chem.* **2004**, *49* (9), 1303–1307. (С. И. Троянов, Н. Б. Шустова, А. А. Попов, М. Файст, Э. Кемниц. Хлорирование фуллеренов C₆₀ и C₇₀ с использованием хлоридов SbCl₅ and VCl₄. *Ж. Неорг. Хим.* **2004**, *49* (9), 1413–1418).
13. A. A. Popov, A. A. Goryunkov, I. V. Goldt, I. S. Kareev, I. V. Kuvychko, W.–D. Hunnius, K. Seppelt, S. H. Strauss, O. V. Boltalina. "Raman, Infrared, and Theoretical Studies of Fluorofullerene C₆₀F₂₀". *J. Phys. Chem. A* **2004**, *108*, 11449-11456. DOI: [10.1021/jp046214a](https://doi.org/10.1021/jp046214a)

2005

14. S. I. Troyanov, N. B. Shustova, A. A. Popov, L. N. Sidorov, E. Kemnitz. "The First Preparation and Structural Characterization of Two Kinetically Stable Chlorofullerenes, C₆₀Cl₂₈ and C₆₀Cl₃₀". *Angew. Chem. Int. Ed.* **2005**, *44*, 432-435. DOI: [10.1002/anie.200462139](https://doi.org/10.1002/anie.200462139)
15. M. V. Korobov, A. G. Bogachev, A. A. Popov, V. M. Senyavin, E. B. Stukalin, A. V. Dzyabchenko, V. A. Davydov, L. S. Kashevarova, A. V. Rakhmanina, V. Agafonov. "Relative stability of polymerized phases of C₆₀: Depolymerization of a tetragonal phase". *Carbon* **2005**, *43*, 954-961. DOI: [10.1016/j.carbon.2004.11.026](https://doi.org/10.1016/j.carbon.2004.11.026)
16. N. B. Shustova, A. A. Popov, L. N. Sidorov, A. P. Turnbull, E. Kemnitz, S. I. Troyanov. "Preparation and crystallographic characterization of C₆₀Cl₂₄". *Chem. Comm.* **2005**, 1411-1413. DOI: [10.1039/B416341A](https://doi.org/10.1039/B416341A)
17. A. B. Kolomeisky, E. B. Stukalin, A. A. Popov. "Understanding mechanochemical coupling in kinesins using first-passage-time processes". *Phys. Rev. E* **2005**, *71*, 031902. DOI: [10.1103/PhysRevE.71.031902](https://doi.org/10.1103/PhysRevE.71.031902)
18. S. I. Troyanov, A. A. Popov. "New [70]Fullerene Chloride, C₇₀Cl₁₆, Obtained by the Attempted Bromination of C₇₀ in TiCl₄". *Angew. Chem. Int. Ed.* **2005**, *44*, 4215-4218. DOI: [10.1002/anie.200500476](https://doi.org/10.1002/anie.200500476)
19. I. V. Kuvychko, A. V. Streletskii, A. A. Popov, S. G. Kotsiris, T. Drewello, S. H. Strauss, O. V. Boltalina. "Seven-Minute Synthesis of Pure C₅-C₆₀Cl₆ from [60]Fullerene and Iodine Monochloride. First IR, Raman, and Mass Spectra of 99 mol% C₆₀Cl₆". *Chem. Eur. J.* **2005**, *11* (18), 5426–5436. DOI: [10.1002/chem.200500185](https://doi.org/10.1002/chem.200500185)
20. M. R. Erenburg, A. A. Popov, O. A. Semenikhin. "Spectroelectrochemical Properties of Some Polymers of Polythiophene Series". *Russian Journal of Electrochemistry* **2005**, *41* (6), 671–680. (М.Р. Эренбург, А.А. Попов, О.А. Семинихин. "Спектроэлектрохимические свойства некоторых полимеров ряда политиофена ". *Электрохимия* **2005**, *41*(6), 755–765.).
21. A. A. Popov, J. Tarabek, I. E. Kareev, S. F. Lebedkin, S. H. Strauss, O. V. Boltalina, L. Dunsch. "Poly(trifluoromethyl)fullerene Radical Anions. An ESR/Vis-NIR Spectroelectrochemical Study of C₆₀F_{2,4} and C₆₀(CF₃)_{2,10}". *J. Phys. Chem. A* **2005**, *109* (43), 9709-9711. DOI: [10.1021/jp0550006](https://doi.org/10.1021/jp0550006)
22. S. I. Troyanov, N. B. Shustova, A. A. Popov, L. N. Sidorov. "Synthesis and Structures of C₆₀ Fullerene Chlorides". *Russ. Chem. Bull., Int. Ed.* **2005**, *7*, 1656 – 1666. (С. И. Троянов, Н. Б.

Шустова, А. А. Попов, Л. Н. Сидоров. "Синтез и строение хлоридов фуллерена C₆₀". *Изв. Акад. Наук., Сер. Хим.* **2005**, 7, 1608-1618.) DOI: 10.1007/s11172-006-0018-4

23. I. E. Kareev, I. V. Kuvychko, A. A. Popov, S. F. Lebedkin, S. M. Miller, O. P. Anderson, S. H. Strauss, O. V. Boltalina. "High-Temperature Synthesis of the Surprisingly Stable C₁-C₇₀(CF₃)₁₀ Isomer with a *para*⁷-*meta*-*para* Ribbon of Nine C₆(CF₃)₂ Edge-Sharing Hexagons". *Angew. Chem. Int. Ed.*, **2005**, 44 (48), 7984-7987 [*Angew. Chem.*, **2005**, 117 (48), 8198-8201]. DOI: 10.1002/anie.200502419

2006

24. E. I. Dorozhkin, D. V. Ignat'eva, N. B. Tamm, A. A. Goryunkov, P. A. Khavrel, I. N. Ioffe, A. A. Popov, I. V. Kuvychko, A. V. Streletskiy, V. Y. Markov, J. Spandl, S. H. Strauss, O. V. Boltalina. "Synthesis, Characterization, and Theoretical Study of Stable Isomers of C₇₀(CF₃)_n (n = 2, 4, 6, 8, 10)". *Chem. Eur. J.* **2006**, 12, 3876 – 3889. DOI: 10.1002/chem.200501346
25. Y. Kobayashi, S. V. Ivanov, A. A. Popov, S. M. Miller, O. P. Anderson, K. A. Solntsev, S. H. Strauss. "Tetrabutylammonium salt of the B₂₄F₂₂⁴⁻ anion. Two B₁₂F₁₁²⁻ icosahedra linked by a 2c-2e B-B bond and surrounded by a sheath of CH₃ · · · FB hydrogen bonds". *Heteroatom Chemistry* **2006**, 17 (3), 181-187. DOI: 10.1002/hc.20220
26. I. E. Kareev, S. F. Lebedkin, A. A. Popov, S. M. Miller, O. P. Anderson, S. H. Strauss, O. V. Boltalina. "1,6,12,15,18,23,25,41,45,57-Decakis(trifluoromethyl)-1,6,12,15,18,23,25,41,45,57-decahydro(C₆₀-I_h)[5,6]fullerene". *Acta Cryst. E* **2006**, E62, o1501–o1503. DOI: 10.1107/S1600536806008300
27. A. A. Popov, V. M. Senyavin, S. I. Troyanov. "Electronic Structure and Spectroscopic Studies of D_{3d}-C₆₀Cl₃₀, a Chlorofullerene with a [18]Trannulene Ring, and Its Relation to Other [18]Trannulenes". *J. Phys. Chem. A* **2006**, 110(23), 7414-7421. DOI: 10.1021/jp060522m
28. A. A. Popov, V. M. Senyavin, O. V. Boltalina, K. Seppelt, J. Spandl, C. S. Feigerle, R. N. Compton. "Infrared, Raman, and DFT Vibrational Spectroscopic Studies of C₆₀F₃₆ and C₆₀F₄₈". *J. Phys. Chem. A* **2006**, 110(28), 8645-8652. DOI: 10.1021/jp060697w
29. M. Krause, A. Popov, L. Dunsch. "Vibrational Structure of Endohedral Fullerene Sc₃N@C₇₈ (D_{3h}') – Evidence for a Strong Coupling between the Sc₃N cluster and C₇₈ Cage". *ChemPhysChem* **2006**, 7 (8), 1734-1740. DOI: 10.1002/cphc.200600139
30. S. Yang, M. Kalbac, A. Popov, L. Dunsch. "Gadolinium-Based Mixed-Metal Nitride Clusterfullerenes Gd_xSc_{3-x}N@C₈₀ (x=1, 2)". *ChemPhysChem* **2006**, 7 (9), 1990-1995. DOI: 10.1002/cphc.200600323
31. M. V. Korobov, A. G. Bogachev, V. M. Senyavin, A. A. Popov, V. A. Davydov, A. V. Rakhmanina, A. V. Markin. "Equilibrium Phase Diagram of Polymerized C₆₀ and Kinetics of Decomposition of the Polymerized Phases *Fullerenes Nanotubes Carbon Nanostr* **2006**, 14 (2-3), 401 – 407. DOI: 10.1080/10407780600665983
32. S. Yang, M. Kalbac, A. Popov, L. Dunsch. "A Facile Route to the Non-IPR Fullerene Sc₃N@C₆₈: Synthesis, Spectroscopic Characterization, and Density Functional Theory Computations (IPR=Isolated Pentagon Rule)". *Chem. Eur. J.* **2006**, 12, 7856 – 7863. DOI: 10.1002/chem.200600261
33. I. E. Kareev, N. B. Shustova, I. V. Kuvychko, S. F. Lebedkin, S. M. Miller, O. P. Anderson, A. A. Popov, S. H. Strauss, O. V. Boltalina, O. V. "Thermally Stable Perfluoroalkylfullerenes with the Skew-Pentagonal-Pyramid Pattern: C₆₀(C₂F₅)₄O, C₆₀(CF₃)₄O, and C₆₀(CF₃)₆". *J. Am. Chem. Soc.* **2006**, 128 (37), 12268-12280. DOI: 10.1021/ja063907r
34. A. A. Goryunkov, I. E. Kareev, I. N. Ioffe, A. A. Popov, I. V. Kuvychko, V. Y. Markov, I. V. Goldt, A. S. Pimenova, M. G. Serov, S. M. Avdoshenko, P. A. Khavrel, L. N. Sidorov, S. F. Lebedkin, Z. Mazej, B. Žemva, S. H. Strauss, O. V. Boltalina. "Reaction of C₆₀ with KMnF₄:

- Isolation and characterization of a new isomer of $C_{60}F_8$ and re-evaluation of the structures of $C_{60}F_7(CF_3)$ and the known isomer of $C_{60}F_8$ ". *J. Fluor. Chem.* **2006**, 1423-1435. DOI: [10.1016/j.jfluchem.2006.06.016](https://doi.org/10.1016/j.jfluchem.2006.06.016)
35. N. B. Shustova, I. V. Kuvychko, R. D. Bolskar, K. Seppelt, S. H. Strauss, A. A. Popov, O. V. Boltalina. "Trifluoromethyl Derivatives of Insoluble Small-HOMO-LUMO-Gap Hollow Higher Fullerenes. NMR and DFT Structure Elucidation of $C_2-(C_{74}-D_{3h})(CF_3)_{12}$, $C_s-(C_{76}-T_d(2))(CF_3)_{12}$, $C_2-(C_{78}-D_{3h}(5))(CF_3)_{12}$, $C_s-(C_{80}-C_{2v}(5))(CF_3)_{12}$, and $C_2-(C_{82}-C_2(5))(CF_3)_{12}$ ". *J. Am. Chem. Soc.* **2006**, 128(49), 15793-15798. DOI: [10.1021/ja0651781](https://doi.org/10.1021/ja0651781)
36. S. Yang, S. I. Troyanov, A. A. Popov, M. Krause, L. Dunsch. "Deviation from the Planarity-a Large Dy_3N Cluster Encapsulated in an I_h-C_{80} Cage: An X-ray Crystallographic and Vibrational Spectroscopic Study". *J. Am. Chem. Soc.* **2006**; 128, 16733-16739. DOI: [10.1021/ja066814i](https://doi.org/10.1021/ja066814i)

2007

37. S. Yang, A. Popov, L. Dunsch. "An Exception to the Isolated Pentagon Rule (IPR): The Endohedral Non-IPR C_{70} Cage of $Sc_3N@C_{70}$ ". *Angew. Chem. Int. Ed.* **2007**, 46 (8), 1256-1259; *Angew. Chem.* **2007**, 119 (8), 1278-1281. DOI: [10.1002/anie.200603281](https://doi.org/10.1002/anie.200603281)
38. M. Krause, F. Ziegls, A. A. Popov, L. Dunsch. "Entrapped Bonded Hydrogen in a Fullerene: the Five-Atom Cluster Sc_3CH in C_{80} ". *ChemPhysChem* **2007**, 8, 537-540. DOI: [10.1002/cphc.200600363](https://doi.org/10.1002/cphc.200600363)
39. A. Popov, M. Krause, S. Yang, J. Wong, L. Dunsch. " C_{78} cage isomerism defined by trimetallic nitride cluster size: a computational and vibrational spectroscopic study". *J. Phys. Chem. B* **2007**, 111, 3363-3369. DOI: [10.1021/jp068661r](https://doi.org/10.1021/jp068661r)
40. I. E. Kareev, N. B. Shustova, D. V. Peryshkov, S. F. Lebedkin, S. M. Miller, O. P. Anderson, A. A. Popov, O. V. Boltalina, S. H. Strauss. "X-ray structure and DFT study of $C_1-C_{60}(CF_3)_{12}$. A high-energy, kinetically-stable isomer prepared at 500 °C". *Chem. Commun.* **2007**, (16), 1650-1652. DOI: [10.1039/B617489B](https://doi.org/10.1039/B617489B)
41. A. M. Lebedev, K. A. Menshikov, V. G. Stankevich, N. Yu. Svechnikov, A. A. Popov, O. V. Boltalina, O. Drozdova, S. Kimura. "Polarized IR studies of $C_{60}F_{18}$ single crystals". *Diamond and Related Materials*, **2007**, 16 (4-7), 1236-1239. DOI: [10.1016/j.diamond.2006.11.093](https://doi.org/10.1016/j.diamond.2006.11.093)
42. N. B. Shustova, B. S. Newell, S. M. Miller, O. P. Anderson, R. D. Bolskar, K. Seppelt, A. A. Popov, O. V. Boltalina, S. H. Strauss. "Discovering and Verifying Elusive Fullerene Cage Isomers: Structures of $C_2-p^{11}-(C_{74}-D_{3h})(CF_3)_{12}$ and $C_2-p^{11}-(C_{78}-D_{3h}(5))(CF_3)_{12}$ ". *Angew. Chem. Int. Ed.* **2007**, 46 (8), 4111-4114. DOI: [10.1002/anie.200604968](https://doi.org/10.1002/anie.200604968)
43. N. B. Shustova, D. V. Peryshkov, A. A. Popov, O. V. Boltalina, S. H. Strauss. 1,6,11,18,24,27,33,51,54,60-Decakis(trifluoromethyl)-1,6,11,18,24,27,33,51,54,60-decahydro($C_{60}-I_h$)[5,6]fullerene. *Acta Cryst. E* **2007**, E63, o3129. DOI: [10.1107/S1600536807026128](https://doi.org/10.1107/S1600536807026128)
44. В. И. Корепанов, А. А. Попов, В. М. Сенявин, М. А. Юровская, Э. С. Чернышова. "ИК спектр и структура 2-тиенил-N-метил-фуллеренопирролидина". *Вестн. Моск. Ун-та. Сер. 2. Химия* **2007**, 48 (2), 86-94.
45. A. A. Popov, I. E. Kareev, N. B. Shustova, E. B. Stukalin, S. F. Lebedkin, K. Seppelt, S. H. Strauss, O. V. Boltalina, L. Dunsch. "Electrochemical, Spectroscopic, and DFT Study of $C_{60}(CF_3)_n$ Frontier Orbitals ($n = 2-18$): The Link between Double Bonds in Pentagons and Reduction Potentials". *J. Am. Chem. Soc.* **2007**, 129 (37), 11551-11568. DOI: [10.1021/ja073181e](https://doi.org/10.1021/ja073181e)

46. N. B. Shustova, A. A. Popov, M. A. Mackey, C. E. Coumbe, J. P. Phillips, S. Stevenson, S. H. Strauss, O. V. Boltalina. "Radical Trifluoromethylation of $\text{Sc}_3\text{N@C}_{80}$ ". *J. Am. Chem. Soc.* **2007**, *129* (38), 11676-11677. DOI: [10.1021/ja074332g](https://doi.org/10.1021/ja074332g)
47. A. A. Popov, L. Dunsch. "Structure, Stability, and Cluster-Cage Interactions in Nitride Clusterfullerenes $\text{M}_3\text{N@C}_{2n}$ (M = Sc, Y; $2n = 68-98$): a Density Functional Theory Study". *J. Am. Chem. Soc.* **2007**, *129* (38), 11835-11549. DOI: [10.1021/ja073809l](https://doi.org/10.1021/ja073809l)
48. Y. Kobayashi, A. A. Popov, S. M. Miller, O. P. Anderson, S. H. Strauss. "Synthesis and Structure of $\text{Ag}(1\text{-Me-}12\text{-SiPh}_3\text{-CB}_{11}\text{F}_{10})$: Selective F12 Substitution in $1\text{-Me-CB}_{11}\text{F}_{11}^-$ and the First $\text{Ag}(\text{arene})_4^+$ Tetrahedron". *Inorg. Chem.* **2007**, *46* (21), 8505-8507. DOI: [10.1021/ic701606p](https://doi.org/10.1021/ic701606p)
49. S. Yang, A. A. Popov, L. Dunsch. "The Role of an Asymmetric Nitride Cluster on a Fullerene Cage: The Non-IPR Endohedral $\text{DySc}_2\text{N@C}_{76}$ ". *J. Phys. Chem. B* **2007**, *111* (49), 13659-13663. DOI: [10.1021/jp709650d](https://doi.org/10.1021/jp709650d)
50. A. A. Popov, I. E. Kareev, N. B. Shustova, S. F. Lebedkin, S. H. Strauss, O. V. Boltalina, L. Dunsch. "Synthesis, Spectroscopic and Electrochemical Characterization, and DFT Study of Seventeen $\text{C}_{70}(\text{CF}_3)_n$ Derivatives ($n = 2, 4, 6, 8, 10, 12$)". *Chem. Eur. J.* **2007**, *14* (1), 107-121. DOI: [10.1002/chem.200700970](https://doi.org/10.1002/chem.200700970)

2008

51. S. Yang, A. A. Popov, M. Kalbac, L. Dunsch. "The Isomers of Gadolinium Scandium Nitride Clusterfullerenes $\text{Gd}_x\text{Sc}_{3-x}\text{N@C}_{80}$ ($x=1, 2$) and Their Influence on Cluster Structure". *Chem. Eur. J.* **2008**, *14* (7), 2084-2092. DOI: [10.1002/chem.200701598](https://doi.org/10.1002/chem.200701598)
52. A. A. Popov, N. B. Shustova, O. V. Boltalina, S. H. Strauss, L. Dunsch. "ESR-Vis/NIR Spectroelectrochemical Study of $\text{C}_{70}(\text{CF}_3)_2^-$ and $\text{C}_{70}(\text{C}_2\text{F}_5)_2^-$ Radical Anions". *ChemPhysChem* **2008**, *9* (3), 431-438. DOI: [10.1002/cphc.200700708](https://doi.org/10.1002/cphc.200700708)
53. S. Yang, A. A. Popov, L. Dunsch. "Large mixed metal nitride clusters encapsulated in a small cage: the confinement of the C_{68} -based clusterfullerenes". *Chem. Commun.* **2008**, 2885-2887. DOI: [10.1039/B803200A](https://doi.org/10.1039/B803200A)
54. P. Rapta, A. A. Popov, S. Yang, L. Dunsch. "The Charged States of $\text{Sc}_3\text{N@C}_{68}$: An in situ Spectroelectrochemical Study of the Radical Cation and Radical Anion of a Non-IPR Fullerene". *J. Phys. Chem. A* **2008**, *112* (26), 5858-5865. DOI: [10.1021/jp802655f](https://doi.org/10.1021/jp802655f)
55. I. E. Kareev, I. V. Kuvychko, N. B. Shustova, S. F. Lebedkin, V. P. Bubnov, O. P. Anderson, A. A. Popov, O. V. Boltalina, S. H. Strauss. " $\text{C}_{1-}(\text{C}_{84}\text{-C}_2(11))(\text{CF}_3)_{12}$: Trifluoromethylation Yields Structural Proof of a Minor C_{84} Cage and Reveals a Principle of Higher Fullerene Reactivity". *Angew. Chem. Int. Ed.* **2008**, *47*, 6204-6207. DOI: [10.1002/anie.200801777](https://doi.org/10.1002/anie.200801777)
56. M. Zalibera, A. A. Popov, M. Kalbac, P. Rapta, L. Dunsch. "The Extended Protocol of the empty $\text{C}_{82:3}$ fullerene cage: Isolation, Structure, Spectroscopy, Electrochemistry, Spectroelectrochemistry and DFT Calculations". *Chem. Eur. J.* **2008**, *14* (32), 9960-9967. DOI: [10.1002/chem.200800591](https://doi.org/10.1002/chem.200800591)
57. S. Yang, A. A. Popov, L. Dunsch. "Carbon Pyramidalization in Fullerene Cages Induced by the Endohedral Cluster: the First Non-Scandium Mixed Metal Nitride Clusterfullerenes". *Angew. Chem. Int. Ed.* **2008**, *47*, 8196-8200. DOI: [10.1002/anie.200802009](https://doi.org/10.1002/anie.200802009)
58. I. E. Kareev, A. A. Popov, I. V. Kuvychko, N. B. Shustova, S. F. Lebedkin, V. P. Bubnov, O. P. Anderson, K. Seppelt, S. H. Strauss, O. V. Boltalina. "Synthesis and X-ray or NMR/DFT Structure Elucidation of Twenty-One New Trifluoromethyl Derivatives of Soluble Cage Isomers of C_{76} , C_{78} , C_{84} , and C_{90} ". *J. Am. Chem. Soc.* **2008**, *130*, 13471-13489. DOI: [10.1021/ja8041614](https://doi.org/10.1021/ja8041614)

59. A. A. Popov, L. Dunsch. "Hindered Cluster Rotation and ^{45}Sc Hyperfine Splitting Constant in Distonoid Anion-Radical $\text{Sc}_3\text{N@C}_{80}^-$, and Spatial Spin-Charge Separation as a General Principle for Anions of Endohedral Fullerenes with Metal-Localized Lowest Unoccupied Molecular Orbital". *J. Am. Chem. Soc.* **2008**, *130* (52), 17726-17742. DOI: [10.1021/ja804226a](https://doi.org/10.1021/ja804226a)

2009

60. A. A. Popov, A. V. Burtsev, V. M. Senyavin, L. Dunsch, S. I. Troyanov. "Spectroscopic and Theoretical Study of the Dimeric Dicationic Fullerene Complex $[(\text{C}_{70})_2]^{2+}(\text{Ti}_3\text{Cl}_{13})^-_2$ ". *J. Phys. Chem. A* **2009**, *113* (1), 263-272. DOI: [10.1021/jp805264q](https://doi.org/10.1021/jp805264q)
61. A. A. Popov, V. M. Senyavin, V. I. Korepanov, I. V. Goldt, A. M. Lebedev, V. G. Stankevich, K. A. Menshikov, N. Yu. Svechnikov, O. V. Boltalina, I. E. Kareev, S. Kimura, O. Sidorova, K. Kanno, I. Akimoto. "Vibrational, electronic, and vibronic excitations of polar $\text{C}_{60}\text{F}_{18}$ molecules: Experimental and theoretical study". *Phys. Rev. B* **2009**, *79* (4), 045413. DOI: [10.1103/PhysRevB.79.045413](https://doi.org/10.1103/PhysRevB.79.045413)
62. A. A. Popov. "Metal-Cage Bonding, Molecular Structures and Vibrational Spectra of Endohedral Fullerenes: Bridging Experiment and Theory". *J. Comput. Theor. Nanosci.* **2009**, *6* (2), 292-317. DOI: [10.1166/jctn.2009.1037](https://doi.org/10.1166/jctn.2009.1037)
63. M. Zalibera, P. Rapta, A. A. Popov, L. Dunsch. "Charged States of Four Isomers of C_{84} Fullerene: In Situ ESR and Vis-NIR Spectroelectrochemistry and DFT Calculations". *J. Phys. Chem. C* **2009**, *113* (13), 5141-5149. DOI: [10.1021/jp811274g](https://doi.org/10.1021/jp811274g)
64. S. Yang, A. A. Popov, C. Chen, L. Dunsch. "Mixed Metal Nitride Clusterfullerenes in Cage Isomers: $\text{Lu}_x\text{Sc}_{3-x}\text{N@C}_{80}$ ($x = 1, 2$) As Compared with $\text{M}_x\text{Sc}_{3-x}\text{N@C}_{80}$ ($\text{M} = \text{Er, Dy, Gd, Nd}$)". *J. Phys. Chem. C* **2009**, *113* (18), 7616-7623. DOI: [10.1021/jp9005263](https://doi.org/10.1021/jp9005263)
65. A. Popov, S. Yang, M. Kalbac, P. Rapta, L. Dunsch. In "Electronic Structure of $\text{Sc}_3\text{N@C}_{68}$ in Neutral and Charged States: An Experimental and TD-DFT Study". In *AIP Conf. Proc.* **1148** "Computational Methods in Science and Engineering, Advances in Computational Science", T. E. Simos and G. Maroulis (Editors), **2009**, pp 712-715. DOI: [10.1063/1.3225413](https://doi.org/10.1063/1.3225413)
66. A. A. Popov, L. Dunsch. "Bonding in Endohedral Metallofullerenes as Studied by Quantum Theory of Atoms in Molecules". *Chem. Eur. J.* **2009**, *15* (38), 9707-9729. DOI: [10.1002/chem.200901045](https://doi.org/10.1002/chem.200901045)
67. S. Yang, C. Chen, A. A. Popov, W. Zhang, F. Liu, L. Dunsch. "An endohedral titanium(III) in a clusterfullerene: putting a non-group-III metal nitride into the $\text{C}_{80}\text{-I}_h$ fullerene cage". *Chem. Commun.* **2009**, 6391-6393. DOI: [10.1039/B803200A](https://doi.org/10.1039/B803200A)
68. N. B. Shustova, Y.-S. Chen, M. A. Mackey, C. E. Coumbe, J. P. Phillips, S. Stevenson, A. A. Popov, O. V. Boltalina, S. H. Strauss. " $\text{Sc}_3\text{N@}(\text{C}_{80}\text{-I}_h(7))(\text{CF}_3)_{14}$ and $\text{Sc}_3\text{N@}(\text{C}_{80}\text{-I}_h(7))(\text{CF}_3)_{16}$. Endohedral Metallofullerene Derivatives with Exohedral Addends on Four and Eight Triple-Hexagon Junctions. Does the Sc_3N Cluster Control the Addition Pattern or Vice Versa?" *J. Am. Chem. Soc.* **2009**, *131* (48), 17630-17637. DOI: [10.1021/ja9069216](https://doi.org/10.1021/ja9069216)
69. D. V. Peryshkov, A. A. Popov, S. H. Strauss. "Direct Perfluorination of $\text{K}_2\text{B}_{12}\text{H}_{12}$ in Acetonitrile Occurs at the Gas Bubble-Solution Interface and Is Inhibited by HF. Experimental and DFT Study of Inhibition by Protic Acids and Soft, Polarizable Anions". *J. Am. Chem. Soc.* **2009**, *131* (51), 18393-18403. DOI: [10.1021/ja9069437](https://doi.org/10.1021/ja9069437)

2010

70. N. B. Shustova, Z. Mazej, Y.-S. Chen, A. A. Popov, S. H. Strauss, O. V. Boltalina. "Saturnene Revealed: X-ray Crystal Structure of $D_{5d}\text{-C}_{60}\text{F}_{20}$ Formed in Reactions of C_{60} with A_xMF_y Fluorinating Agents ($\text{A} = \text{Alkali Metal}$; $\text{M} = 3d \text{ Metal}$)". *Angew. Chem. Int. Ed.* **2010**, *49*, 812-815. DOI: [10.1002/anie.200905832](https://doi.org/10.1002/anie.200905832)

71. X.-B. Wang, C. Chi, I. V. Kuvychko, K. Seppelt, A. A. Popov, S. H. Strauss, O. V. Boltalina, L.-S. Wang. "Photoelectron Spectroscopy of $C_{60}F_n^-$ and $C_{60}F_m^{2-}$ ($n = 17, 33, 35, 43, 45, 47$; $m = 34, 46$) in the Gas Phase and the Generation and Characterization of $C_1-C_{60}F_{47}^-$ and $D_2-C_{60}F_{44}$ in Solution". *J. Phys. Chem. A* **2010**, *114*, 1756-1765. DOI: [10.1021/jp9097364](https://doi.org/10.1021/jp9097364)
72. A. A. Popov, L. Zhang, L. Dunsch. "A pseudoatom in a cage: trimetallofullerene $Y_3@C_{80}$ mimics $Y_3N@C_{80}$ with nitrogen substituted by a pseudoatom". *ACS Nano* **2010**, *4*(2), 795-802. DOI: [10.1021/nn901422z](https://doi.org/10.1021/nn901422z)
73. L. Dunsch, S. Yang, L. Zhang, A. Svitova, S. Oswald, A. A. Popov. "Metal Sulfide in a C_{82} Fullerene Cage: A New Form of Endohedral Clusterfullerenes". *J. Am. Chem. Soc.* **2010**, *132*, 5413-5421. DOI: [10.1021/ja909580j](https://doi.org/10.1021/ja909580j)
74. N. Chen, S. Klod, P. Rapta, A. A. Popov, L. Dunsch. "Direct Arc-Discharge Assisted Synthesis of $C_{60}H_2(C_3H_5N)$: A cis-1-Pyrrolino C_{60} Fullerene Hydride with Unusual Redox Properties". *Chem. Mater.* **2010**, *22* (8), 2608-2615. DOI: [10.1021/cm903870v](https://doi.org/10.1021/cm903870v)
75. A. Vargová, A. A. Popov, P. Rapta, B. Sun, L. Zhang, L. Dunsch. "Electrochemical Tuning of Spin States of the Endohedral Metallofullerene $Y@C_{82}$ as Probed by ESR Spectroelectrochemistry". *ChemPhysChem*, **2010**, *11*, 1650-1653. DOI: [10.1002/cphc.200901015](https://doi.org/10.1002/cphc.200901015)
76. A. A. Popov, N. B. Shustova, A. L. Svitova, M. A. Mackey, C. E. Coumbe, J. P. Phillips, S. Stevenson, S. H. Strauss, O. V. Boltalina, L. Dunsch. "Redox tuning endohedral fullerene spin states. From the dication to the trianion radical of $Sc_3N@C_{80}(CF_3)_2$ in five reversible single-electron steps". *Chem. Eur. J.* **2010**, *16* (16), 4721-4724. DOI: [10.1002/chem.201000205](https://doi.org/10.1002/chem.201000205). *Inside cover* DOI: [10.1002/chem.201090074](https://doi.org/10.1002/chem.201090074)
77. I. V. Kuvychko, A. V. Streletskii, N. B. Shustova, K. Seppelt, T. Drewello, A. A. Popov, S. H. Strauss, O. V. Boltalina. "Soluble Chlorofullerenes $C_{60}Cl_{2,4,6,8,10}$. Synthesis, Purification, Compositional Analysis, Stability, and Experimental/Theoretical Structure Elucidation, Including the X-ray Structure of $C_{1-1,2,7,10,14,24,25,28,29,31}-C_{60}Cl_{10}$ ". *J. Am. Chem. Soc.* **2010**, *132* (18), 6443-6462. DOI: [10.1021/ja1005256](https://doi.org/10.1021/ja1005256)
78. L. Zhang, A. A. Popov, S. Yang, S. Klod, P. Rapta, L. Dunsch. "An endohedral redox system in a fullerene cage: the Ce based mixed-metal cluster fullerene $Lu_2CeN@C_{80}$ ". *Phys. Chem. Chem. Phys.* **2010**, *12*, 7840-7847. DOI: [10.1039/c002918a](https://doi.org/10.1039/c002918a). *Inside cover* DOI: [10.1039/C0CP90047H](https://doi.org/10.1039/C0CP90047H)
79. A. A. Popov, C. Chen, S. Yang, F. Lipps, L. Dunsch. "The Spin-Flow Vibrational Spectroscopy of Molecules with Flexible Spin Density: Electrochemistry, ESR, Cluster and Spin Dynamics, and Bonding in $TiSc_2N@C_{80}$ ". *ACS Nano* **2010**, *4* (8), 4857-4871. DOI: [10.1021/nn101115d](https://doi.org/10.1021/nn101115d)
80. A. A. Popov, I. E. Kareev, N. B. Shustova, S. H. Strauss, O. V. Boltalina, L. Dunsch. "Unraveling the Electron Spin Resonance Pattern of Nonsymmetric Radicals with 30 Fluorine Atoms: Electron Spin Resonance and Vis-Near-Infrared Spectroelectrochemistry of the Anion Radicals and Dianions of $C_{60}(CF_3)_{2n}$ ($2n = 2-10$) Derivatives and Density Functional Theory-Assisted Assignment." *J. Am. Chem. Soc.* **2010**, *132* (33), 11709-11721. DOI: [10.1021/ja1043775](https://doi.org/10.1021/ja1043775)
81. D. Peryshkov, A. A. Popov, S. H. Strauss. "Latent Porosity in Potassium Dodecafluoro-closododecaborate(2-). Structures and Rapid Room Temperature Interconversions of Crystalline $K_2B_{12}F_{12}$, $K_2(H_2O)_2B_{12}F_{12}$, and $K_2(H_2O)_4B_{12}F_{12}$ in the Presence of Water Vapor". *J. Am. Chem. Soc.* **2010**, *132* (39), 13902-13913. DOI: [10.1021/ja105522d](https://doi.org/10.1021/ja105522d)
82. N. B. Shustova, I. E. Kareev, I. V. Kuvychko, J. B. Whitaker, S. F. Lebedkin, A. A. Popov, L. Dunsch, Y.-S. Chen, K. Seppelt, S. H. Strauss, O. V. Boltalina. "High-temperature and

photochemical syntheses of C₆₀ and C₇₀ fullerene derivatives with linear perfluoroalkyl chains". *J. Fluor. Chem.* **2010**, *131*, 1198-1212. DOI: [10.1016/j.jfluchem.2010.08.001](https://doi.org/10.1016/j.jfluchem.2010.08.001)

83. I. V. Kuvychko, A. A. Popov, A. V. Streletskii, L. C. Nye, T. Drewello, S. H. Strauss, O. V. Boltalina. "Dynamic HPLC study of C₇₀ chlorination reveals a surprisingly selective synthesis of C₇₀Cl₈". *Chem. Commun.* **2010**, *46*, 8204-8206. DOI: [10.1039/C0CC03134H](https://doi.org/10.1039/C0CC03134H)

2011

84. N. B. Shustova, I. V. Kuvychko, D. V. Peryshkov, J. B. Whitaker, B. W. Larson, Y.-S. Chen, L. Dunsch, K. Seppelt, A. A. Popov, S. H. Strauss, O. V. Boltalina. "Chemical tailoring of fullerene acceptors: synthesis, structures and electrochemical properties of perfluoroisopropylfullerenes." *Chem. Commun.* **2011**, *47*, 875-877. DOI: [10.1039/C0CC03247F](https://doi.org/10.1039/C0CC03247F)
85. N. B. Shustova, D. V. Peryshkov, I. V. Kuvychko, Y.-S. Chen, M. A. Mackey, C. E. Coumbe, D. T. Heaps, B. S. Confait, T. Heine, J. P. Phillips, S. Stevenson, L. Dunsch, A. A. Popov, S. H. Strauss, O. V. Boltalina. "Poly(perfluoroalkylation) of Metallic Nitride Fullerenes Reveals Addition-Pattern Guidelines: Synthesis and Characterization of a Family of Sc₃N@C₈₀(CF₃)_n (n = 2-16) and Their Radical Anions." *J. Am. Chem. Soc.* **2011**, *133* (8), 2672-2690. DOI: [10.1021/ja109462j](https://doi.org/10.1021/ja109462j)