

Natalia Shustova

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Professional Appointments and Education

Fred M. Weissman Palmetto Professor	2023–present
Executive Committee for the Beckman Foundation	2023–present
Cottrell Scholar Selection Committee	2022–present
Associate Editor, ACS Materials Letters	2022–present
Professor	2021–present
Chair of the International MOF Commission	2024–present
IAS Hans Fischer Fellow, Technical University of Munich	2020–present
Peter and Bonnie McCausland Associate Professor	2019–2020
Associate Professor of Chemistry, University of South Carolina	2018–2020
Associate Editor, Materials Chemistry Frontiers	2016–2019
Assistant Professor of Chemistry, University of South Carolina	2013–2017
Postdoctoral Associate, Massachusetts Institute of Technology	2010–2013
Ph.D. in Inorganic Chemistry, Colorado State University	2005–2010
Ph.D. in Physical Chemistry, Moscow State University	2004–2005

Awards and Honors

SC ACS Outreach Volunteer of the Year	2026
Distinguished Research Service Award	2026
Friedrich Wilhelm Bessel Research Award, The Alexander von Humboldt Foundation	2023
Russel Research Award	2023
IAS Hans Fischer Fellowship	2020
Camille Dreyfus Teaching-Scholar Award	2019
McCausland Fellowship	2019
Distinguished Undergraduate Research Mentor Award	2019
Alfred P. Sloan Research Award	2017
Cottrell Scholar Award – Research Corporation for Science Advancement	2017
Breakthrough Award	2017
Scialog Fellow, Research Corporation for Science Advancement	2017
NSF CAREER Award	2016
MIT Infinite Kilometer Postdoctoral Award	2013
MIT/Bruker Symposium Poster Award	2013
Graduate Teaching Assistant Award, Colorado State University	2009
XIX International Symposium on Fluorine Chemistry Poster Award (first prize)	2009
German Academic Exchange Service (DAAD) Scholarship	2009
ECS Poster Award	2009
Herbert H. Uhlig ECS Summer Fellowship	2008
ECS Solid-State Science and Technology Poster Award	2008
AWIS Educational Foundation Citation of Merit	2008
International J. Soros Science Education Program Fellowship	2002, 2005
L. Euler Student Fellowship	2003, 2004
V. F. Luginin Research Award, Moscow State University	2002, 2003
International Student Conference (first prize), Moscow State University	2002–2004

Book and Book Chapters

- 1. Handbook of Metal-Organic Frameworks: Synthesis and Characterization Methods** (Shustova N. B. and Li J.), World Scientific, **2026**.
- 2. Chapter 4:** Perfluoroalkylation of Fullerenes, *Handbook of Carbon Nano Materials* (Editors: D'Souza, F. and Kadish, K. M.), World Scientific, **2011**, pp. 102–135.
- 3. Chapter 68:** High-Yield Synthesis of a Single Asymmetric Isomer of C₇₀(CF₃)₁₀ by High Temperature Radical Trifluoromethylation *Efficient Preparation of Fluorine Compounds*, (Editor: Roesky, H. W.), John Wiley and Sons, Inc., **2013**.

Publications (* denotes Shustova, N. as a corresponding author)

130. Thaggard, G. C.; Smith, D. N.; Basak, S.; Maldeni Kankanamalage, B. K. P.; Morris, A. J.*; **Shustova, N. B.*** "Building Chemistry from "Lego" Blocks: Metal–Organic Frameworks after the 2025 Nobel Prize" *ACS Cent. Sci.* **2026**, *12*, 941–950.
129. Naik, M.; Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Smith, D. N.; Martin, C. R.; Lim, J.; Gevorgyan, V.; Karakalos, S. G.; Smith, M. D.; Garashchuk, S.; **Shustova, N. B.*** "Stimuli-Modulated Metal–Organic Framework (MOF) Reactivity toward a Three-Component Coupling Reaction" *J. Am. Chem. Soc.* **2026**, *148*, 22240–22252.
128. Thaggard, G. C.; Smith, D. N.; Maldeni Kankanamalage, B. K. P.; Jentz, S. M. **Shustova, N. B.*** "Thermodynamics of Metal–Organic Frameworks: From Fundamentals to Advanced Applications" *Chem. Soc. Rev.* **2026**, *55*, 5707–5727.
127. Maldeni Kankanamalage, B. K. P.; Thompson, W. J.; Smith, D. N.; Thaggard, G. C.; Wijerathne, N.; Incognito, I.; Byers, J. A.; Niu, J.*; **Shustova, N. B.*** "Catalyst Hide-and-Seek Beneath Porous Support Surfaces: Pinpointing Active Site Distribution Through Resonance Energy Transfer" *Angew. Chem. Int. Ed.* **2026**, e4042285.
126. Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Lim, J.; Shi, X.; Arnold, V. S.; Badiger, M.; Mulkerrin, R.; Broskey, R. D.; Irizarry, E.; Atim, G.; Azmy, A.; Smith, M. D.; Garashchuk, S.; Spanopoulos, I.; **Shustova, N. B.*** "Altering the Thermodynamics of Stimuli-Responsive Derivatives through Layered Hybrid Material Design" *J. Am. Chem. Soc.* **2025**, *147*, 42591–42606.
125. Haimerl, J.; Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Bühler, R.; Lim, J.; Park, K. C.; Warnan, J.; Fischer, R. A.; **Shustova, N. B.*** "Shifting Gears: Photochromic Metal–Organic Frameworks with Stimulus-Adaptable Performance" *J. Am. Chem. Soc.* **2025**, *147*, 19918–19930.
124. Park, K. C.; Lim, J.; Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Lehman-Andino, I.; Liu, Y.; Burrell, J. M.; Martin, C. R.; Ta, A. T.; Greytak, A. B.; Amoroso, J. W.; DiPrete, D. D.; Smith, M. D.; Phillpot, S. R.; **Shustova, N. B.*** "Stimuli-Responsive Photoswitch-Actinide Binding: A Match Made in MOFs" *Chem. Sci.* **2025**, *16*, 14115–14126 (**selected as "Pick of the Week" paper and highlighted in the 2025 HOT Article Collection**).
123. Thaggard, G. C.; **Shustova, N. B.*** "COFs in the Game: Harvest Water to Sustain" *ACS Central Sci.* **2025**, *11*, 653–655.
122. Thaggard, G. C.; Wilson, G. R.; Naik, M.; Quetel, M. A.; Lim, J.; Maldeni Kankanamalage, B. K. P.; Smith, M. D. **Shustova, N. B.*** "A Change of Pace: Record Photoresponse through Spirooxazine Confinement in a Metal–Organic Matrix" *J. Am. Chem. Soc.* **2024**, *146*, 31746–31756.
121. Lim, J.; Park, K. C.; Thaggard, G. C.; Liu, Y.; Maldeni Kankanamalage, B. K. P.; Toler, D. J.; Ta, A. T.; Kittikhunnatham, P.; Smith, M. D.; Phillpot, S. R.; **Shustova, N. B.*** "Friends or Foes: Fundamental Principles of Th–Organic Scaffold Chemistry Using Zr-analogs as a Guide" *J. Am. Chem. Soc.* **2024**, *146*, 12155–12166.
120. Park, K. C.; Lim, J.; Thaggard, G. C.; **Shustova, N. B.*** "Mining for Metal–Organic Systems: Chemistry Frontiers of Th-, U-, and Zr-Materials" *J. Am. Chem. Soc.* **2024**, *146*, 18189–18204.
119. Maldeni Kankanamalage, B. K. P.; Thompson, W. J.; Thaggard, G. C.; Park, K. C.; Martin, C. R.; Niu, J.; Byers, J.A.; **Shustova, N. B.*** "Catalytically Active Site Mapping Realized through Energy Transfer Modeling" *Angew. Chem. Int. Ed.* **2024**, e202416695.
118. Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Park, K. C.; Lim, J.; Quetel, M. A.; Naik, M.; **Shustova, N. B.*** "Switching from Molecules to Functional Materials: Breakthroughs in Photochromism with MOFs" *Adv. Mater.* **2024**, 2410067.
117. Thaggard, G. C.; Maldeni Kankanamalage, B. K. P.; Park, K. C.; Haimerl, J.; Fischer, R. A.; **Shustova, N. B.*** "Switching in Harmony: Tailoring the Properties of Functional Materials with Orthogonal Stimuli" *Chem. Phys. Rev.* **2024**, *5*, 011305 (**selected as a Featured Article and highlighted on the cover**).
116. Martin, C. R.; Thaggard, G. C.; Lehman-Andino, I.; Mollinedo, E.; Rai, B. K.; Page, M. A.; Taylor-Pashow, K.; Shustova, N. B. "Photochromic Ln-MOFs: A Platform for Metal-Photoswitch Cooperativity" *Inorg. Chem.* **2024**, *63*, 12810–12817.
115. Thaggard, G. C.; Park, K. C.; Lim, J.; Maldeni Kankanamalage, B. K. P.; Haimerl, J.; Wilson, G. R.; McBride, M. K.; Forrester, K. L.; Adelson, E. R.; Arnold, V. S.; Wetthasinghe, S. T.; Rassolov, V. A.; Smith, M. D.; Sosnin, D.; Aprahamian, I.; Karmakar, M.; Bag, S. K.; Thakur, A.; Zhang, M.; Tang, B. Z.; Castaño, J. A.; Chaur, M. N.; Lerch, M. M.; Fischer, R. A.; Aizenberg, J.; Herges, R.; Lehn, J.-M.; **Shustova, N. B.*** "Breaking the Photoswitch Speed Limit" *Nat. Commun.* **2023**, *14*, 7556.
114. **Shustova, N. B.*** "Anthracene-based Energy Storage" *Joule* **2024**, *8*, 2957–2959 (invited).
113. Wilson, G. R.; Park, K. C.; Thaggard, G. C.; Martin, C. R.; Hill, A. R.; Haimerl, J.; Lim, J.; Maldeni Kankanamalage, B. K. P.; Yarbrough, B.; Forrester, K. L.; Fischer, R. A.; Pellechia, P. J.; Smith, M. D.; Garashchuk, S.; **Shustova, N. B.*** "Cooperative and Orthogonal Switching in the Solid State Enabled by Metal–Organic Framework Confinement Leading to a Thermo-Photochromic Platform" *Angew. Chem. Int. Ed.* **2023**, e202308715 (**VIP paper**).
112. Thaggard, G. C.; Haimerl, J.; Fischer, R. A.; Park, K. C.; **Shustova, N. B.*** "Traffic Lights for Catalysis: Stimuli-Responsive Molecular and Extended Catalytic Systems" *Angew. Chem. Int. Ed.* **2023**, e202302859.
111. Thaggard, G. C.; Haimerl, J.; Park, K. C.; Lim, J.; Fischer, R.; Maldeni Kankanamalage, B. K. P.; Yarbrough, B. J.; Wilson, G. R.; **Shustova, N. B.*** "Metal-Photoswitch Friendship: From Photochromic Complexes to Functional Materials" *J. Am. Chem. Soc.* **2022**, *51*, 23249–23263.

110. Park, K. C.; Kittikhunnatham, P.; Lim, J.; Thaggard, G. C.; Liu, Y.; Martin, C. R.; Leith, G. A.; Toler, D. J.; Ta, A. T.; Birkner, N.; Lehman-Andino, I.; Hernandez-Jimenez, A.; Morrison, G.; Amoroso, J. W.; zur Loye, H.-C.; DiPrete, D. P.; Smith, M. D.; Brinkman, K. S.; Phillpot, S. R.; **Shustova, N. B.*** "The Highly Operational Team (HOT) toward *f*-block Materials" *Angew. Chem. Int. Ed.* **2023**, 62, e202307093.
109. Park, K. C.; Kittikhunnatham, P.; Lim, J.; Thaggard, G. C.; Liu, Y.; Martin, C. R.; Leith, G. A.; Toler, D. J.; Ta, A. T.; Birkner, N.; Lehman-Andino, I.; Hernandez-Jimenez, A.; Morrison, G.; Amoroso, J. W.; zur Loye, H.-C.; DiPrete, D. P.; Smith, M. D.; Brinkman, K. S.; Phillpot, S. R.; **Shustova, N. B.*** "*f*-block MOFs: A Pathway to Heterometallic Transuranics" *Angew. Chem. Int. Ed.* **2023**, 62, e202216349.
108. Thaggard, G. C.; Leith, G. A.; Sosnin, D.; Martin, C. R.; Park, K. C.; McBride, M. K.; Lim, J.; Yarbrough, B. J.; Maldeni Kankanamalage, B. K. P.; Wilson, G. R.; Hill, A. R.; Smith, M. D.; Garashchuk, S.; Greytak, A. B.; Aprahamian, I.; **Shustova, N. B.*** "Confinement-Driven Photophysics in Hydrazone-based Hierarchical Materials" *Angew. Chem. Int. Ed.*, **2023**, 62, e202211776 (**VIP paper**).
107. Kwon, J.; Ma, H.; Giri, A.; Hopkins, P.; **Shustova, N. B.**; Tian, Z. "Thermal Conductivity of Covalent Organic Frameworks" *ACS Nano* **2023**, 17, 15222–15230.
106. Park, K. C.; Martin, C. R.; Leith, G. A.; Thaggard, G. C.; Wilson, G. R.; Yarbrough, B. J.; Maldeni Kankanamalage, B. K. P.; Kittikhunnatham, P.; Mathur, A.; Jatoi, I.; Manzi, M. A.; Lim, J.; Lehman-Andino, I.; Hernandez-Jimenez, A.; Amoroso, J. W.; DiPrete, D. P.; Liu, Y.; Schaeperkoetter, J.; Misture, S. T.; Phillpot, S. R.; Hu, S.; Li, Y.; Leydier, A.; Proust, V.; Grandjean, A.; Smith, M. D.; **Shustova, N. B.*** "Capture Instead of Release: Defect-Modulated Radionuclide Leaching Kinetics in Metal-Organic Frameworks" *J. Am. Chem. Soc.* **2022**, 144, 16139–16149.
105. Stanley, P. M.; Haimerl, J.; **Shustova, N. B.**; Fischer, R. A.; Warnan, J. "Merging Molecular Catalysts and Metal–Organic Frameworks for Photocatalytic Fuel Production" *Nat. Chem.* **2022**, 14, 1342–1356.
104. Leith, G. A.; **Shustova, N. B.*** "Keeping COFs in the loop" *Nat. Chem.* **2022**, 14, 485–486.
103. Martin, C. R.; Park, K. C.; Leith, G. A.; Yu, J.; Mathur, A.; Wilson, G. R.; Gange, G. B.; Barth, E. L.; Ly, R. T.; Manley, O. M.; Forrester, K. L.; Karakalos, S. G.; Smith, M. D.; Makris, T. M.; Vannucci, A. K.; Peryshkov, D. V.; **Shustova, N. B.*** "Stimuli-Modulated Metal Oxidation States in Photochromic MOFs" *J. Am. Chem. Soc.* **2022**, 144, 4457–4468 (**highlighted on the cover**).
102. Leith, G. A.; Martin, C. R.; Park, K. C.; **Shustova, N. B.*** "Playing "Jenga" with MOFs: De-interpenetration for Pore Opening" *Chem.* **2022**, 14, 485–486.
101. Faillace, M. S.; Dolgoplova, E. A.; Ceballos, N. M.; Ruiz Pereyra, E. N.; Lanfri, L.; Argüello, G. A.; Paci, M. B.; **Shustova, N. B.**; Peláez, W. J. "GFP-related Chromophores: Photoisomerization, Thermal Reversion, and DNA Labeling" *Phys. Chem. Chem. Phys.* **2023**, 25, 17943–17951.
100. Liu, Y.; Ta, A. T.; Pandey, S.; Park, K. C.; Hu, S.; Shustova, N. B.; Phillpot, S. R. "Binding of Uranyl Cations to a Zr-based Metal-Organic Framework by Density Functional Theory" *Comput. Mat. Sci.* **2023**, 230, 112528.
99. Faillace, M. S.; Ceballos, N. M.; Shustova, N. B.; Peláez, W. J. "Selective Synthesis using ETFBO: A New Strategy for the Preparation of Hexahydro-1H-pyrrolo[1,2-*c*]imidazol-1-one" *Asian J. Org. Chem.* **2023**, e202300318.
98. Kittikhunnatham, P.; Leith, G. A.; Mathur, A.; Naglic, J. K.; Martin, C. R.; Park, K. C.; McCullough, K.; Jayaweera, C. H. D. A.; Corkill, R. E.; Lauterbach, J.; Karakalos, S. G.; Smith, M. D.; Garahschuk, S.; Chen, D. A.; **Shustova, N. B.*** "A MOF Multifunctional Cargo Vehicle for Reactive-Gas Delivery and Catalysis" *Angew. Chem. Int. Ed.* **2022**, 61, e20211390.
97. Martin, C. R.; Leith, G. A.; Kittikhunnatham, P.; Park, K. C.; Ejegbavwo, O. A.; Mathur, A.; Callahan, C. R.; Desmond, S. L.; Keener, M. R.; Ahmed, F.; Pandey, S.; Smith, M. D.; Phillpot, S. R.; Greytak, A. B.; **Shustova, N. B.*** "Heterometallic Actinide-Containing Photoresponsive Metal-Organic Frameworks: Dynamic and Static Tuning of Electronic Properties" *Angew. Chem. Int. Ed.* **2021**, 60, 8072–8080 (**article featured as a frontispiece; Metal-Organic Frameworks: Special Collection**).
96. Chen, D. A.; Jimenez, J. D.; Senanayake, S. D.; Stetzler, J. P.; Shakya, D. M.; Mcarver, G. A.; Rajeshkumar, T.; Vogiatzis, K. D.; Mathur, A.; **Shustova, N. B.**; Myrick, M. L.; Metavarayuth, K.; Royko, M. M.; Lauterbach, J.; Tate, G. L.; Monnier, J. R. "Mechanistic Investigations of Gas-Phase Catalytic Hydrogenation in Metal-Organic Frameworks: Cooperative Activity of the Metal and Linker Sites in Cu_xRh_{3-x}(BTC)₂" *J. Phys. Chem. C.* **2022**, 60, 11553–11565.
95. Leith, G. A.; **Shustova, N. B.*** "Graphitic Supramolecular Architectures Based on Corannulene, Fullerene, and Beyond" *Chem. Comm.* **2021**, 57, 10125–10138 (**invited**).
94. Stanley, P. M.; Haimerl, J.; Thomas, C.; Urstoeger, A.; Schuster, M.; **Shustova, N. B.**; Casini, A.; Rieger, B.; Warnan, J.; Fischer, R. A. "Host-Guest Interactions in Metal-Organic Framework Isorecticular Series for Molecular Photocatalytic CO₂ Reduction" *Angew. Chem. Int. Ed.* **2021**, 60, 17854–17860 (**highlighted on the cover**).
93. Martin, C. R.; Leith, G. A.; **Shustova, N. B.*** "Beyond Structural Motifs: The Frontier of Actinide-Containing Metal-Organic Frameworks" *Chem. Sci.* **2021**, 12, 7214–7230 (**invited**).

92. Leith, G. A.; Martin, C. R.; Mathur, A.; Kittikhunnatham, P.; Park, K. C.; **Shustova, N. B.*** "Dynamically-Controlled Electronic Behavior of Stimuli-Responsive Materials: Exploring Dimensionality and Connectivity" *Adv. Energy Mater.* **2022**, *12*, 2100441 (**special Issue: "Dimensionality, Emerging Materials, and Energy"**).
91. Martin, C. R.; Park, K. C.; Corkill, R. E.; Kittikhunnatham, P.; Leith, G. A.; Mathur, A.; Abiodun, S. L.; Greytak, A. B.; **Shustova, N. B.*** "Photoresponsive Frameworks: Energy Transfer in the Spotlight" *Faraday Discuss.*, **2021**, *231*, 266–280 (**invited contribution as a part of a Faraday Discussion Series: "MOFs for Energy and the Environment"**).
90. Leith, G. A.; Rice, A. M.; Yarbrough, B. J.; Kittikhunnatham, P.; Mathur, A.; Morris, N. A.; Francis, M. J.; Berseneva, A. A.; Dhull, P.; Adams, R. D.; Bobo, M. V.; Vannucci, A. A.; Smith, M. D.; Garashchuk, S.; **Shustova, N. B.*** "Broken-Hearted" Carbon Bowl via Electron Shuttle Reaction: Energetics and Electron Coupling" *Chem. Sci.* **2021**, *12*, 6600–6606.
89. Li, Y.; Hu, S.; Hilty, F. W.; Montgomery, R.; Park, K. C.; Martin, C. R.; **Shustova, N. B.**; Liu, Y.; Phillpot, S. R. "Leaching Model of Radionuclides in Metal-Organic Framework Particles" *Comput. Mater. Sci.* **2022**, *201*, 110886.
88. Leith, G. A.; Martin, C. R.; Mayers, J.; Kittikhunnatham, P.; Larsen, R.; **Shustova, N. B.***; "Confinement-Guided Photophysics in MOFs, COFs, and Cages" *Chem. Soc. Rev.* **2021**, *50*, 4382–4410. (**themed collection of Chemical Society Reviews on "Nanoconfinement"**)
87. **Shustova, N. B.*** "Natalia Shustova answers questions about 15 years of research on covalent organic frameworks" *Nat. Commun.* **2020**, *11*, 5329.
86. Dolgoplova, E. A.; Berseneva, A. A.; Faillace, M. S.; Ejegbavwo, O. A.; Leith, G. A.; Choi, S. W.; Gregory, H. N.; Rice, A. M.; Smith, M. D.; Chruszcz, M.; Garashchuk, S.; Mythreye, K.; **Shustova, N. B.*** "Confinement-Driven Photophysics in Cages, Covalent-Organic Frameworks, Metal-Organic Frameworks, and DNA" *J. Am. Chem. Soc.* **2020**, *142*, 4769–4783.
85. Leith, G. A.; Rice, A. M.; Yarbrough, B. J.; Berseneva, A. A.; Ly, R. T.; Buck, C. N. III; Chusov, D.; Brandt, A. J.; Chen, D. A.; Lamm, B. W.; Stefik, M.; Stephenson, K. S.; Smith, M. D.; Vannucci, A. K.; Pellechia, P. J.; Garashchuk, S.; **Shustova, N. B.*** "A Dual Threat: Redox-Activity and Electronic Structures of Well-Defined Donor-Acceptor Fullerene Covalent-Organic Materials" *Angew. Chem. Int. Ed.* **2020**, *59*, 6000–6009.
84. Ejegbavwo, O. E.; Berseneva, A. A.; Martin, C. R.; Leith, G. A.; Pandey, S.; Brandt, A. J.; Park, K. C.; Mathur, A.; Farzandh, S.; Klepov, V. V.; Heiser, B. J.; Chandrashekar, M.; Karakalos, S. G.; Smith, M. D.; Phillpot, S. R.; Garashchuk, S.; Chen, D. A.; **Shustova, N. B.*** "Heterometallic Multinuclear Nodes Directing MOF Electronic Behavior" *Chem. Sci.* **2020**, *11*, 7379–7389.
83. Martin, C. R.; Kittikhunnatham, P.; Leith, G. A.; Berseneva, A. A.; Park, K. C.; Greytak, A. B.; **Shustova, N. B.*** "Let the Light be a Guide: Chromophore Communication in Metal-Organic Frameworks" *Nano Res.* **2021**, *14*, 338–354 (**special issue: Future Directions of Reticular Chemistry**).
82. Metavarayuth, K.; Ejegbavwo, O. A.; McCarver, G.; Myrick, M.; Makris, T.; Vogiatzis, K.; Senanayake, S.; Manley, O.; Ebrahim, A.; Frenkel, A.; Hwang, S.; Rajeshkumar, T.; Jimenez, J.; Chen, K.; **Shustova, N. B.***; Chen, D. A. "Direct Identification of Mixed-Metal Centers in Metal-Organic Frameworks: Cu₃(BTC)₂ Transmetalated with Rh²⁺ Ions" *Phys. Chem. Lett.* **2020**, *11*, 8138–8144.
81. Pandey, S.; Demaske, B.; Ejegbavwo, O. A.; Berseneva, A. A.; Setyawan, W.; Shustova, N. B.; Phillpot, S. "Electronic Structures and Magnetism of Zr-, Th-, and U-based Metal-Organic Frameworks (MOFs) by Density Functional Theory" *Comput. Mater. Sci.* **2020**, *184*, 109903.
80. Brandt, A. J.; Shukla, D.; Metavarayuth, K.; Dolgoplova, E.; Hensley, L.; Duke, A. S.; Farzandh, S.; Stefik, M.; **Shustova, N. B.***; Chen, D. A. "Growth of Crystalline Bimetallic Metal-Organic Framework Films via Transmetalation" *Langmuir* **2020**, *36*, 9900–9908.
79. Li, D.; Shustova, N. B.; Martin, C. R.; Taylor-Pashow, K.; Seaman, J. C.; Kaplan, D. I.; Amoroso, J. W.; Chernikov, R. J. Anion-Exchanged and Quaternary Ammonium Functionalized MIL-101-Cr Metal-Organic Framework (MOF) for ReO⁻/TcO⁻ Sequestration from Groundwater *Environ. Radioact.* **2020**, *222*, 106372.
78. Ejegbavwo, O. A.; Martin, C. R.; Oyindamola, A. O.; Leith, G. A.; Ly, R. T.; Rice, A. M.; Dolgoplova, E. A.; Smith, M. D.; Karakalos, S. G.; Birkner, N.; Powell, B. A.; Pandey, S.; Koch, R. J.; Mixture, S. T.; zur Loye, H.-C.; Phillpot, S. R.; Brinkman, K. S.; Shustova, N. B. "Thermodynamics and Electronic Properties of Heterometallic Multinuclear An-MOFs with "Structural Memory"" *J. Am. Chem. Soc.* **2019**, *141*, 11628–11640 (**highlighted on the cover**).
77. Leith, G. A.; Berseneva, A. A.; Mathur, A.; Park, K. C.; **Shustova, N. B.*** "A Multivariate Toolbox for Donor-Acceptor Alignment: MOFs and COFs" *Trends Chem.* **2020**, *2*, 367–382. (**highlighted in the special issue: First Anniversary-Laying Groundwork for the Future; the editor's choice of Trends in Chemistry papers**).
76. Rice, A. M.; Martin, C. R.; Galitskiy, V. A.; Berseneva, A. A.; Leith, G. A.; **Shustova, N. B.*** "Photophysics Modulation in Photoswitchable Metal-Organic Frameworks" *Chem. Rev.* **2020**, *120*, 8790–8813.
75. Berseneva, A. A.; Martin, C. R.; Galitskiy, V. A.; Ejegbavwo, O. A.; Ly, R. T.; Rice, A. M.; Dolgoplova, E. A.; Smith, M. D.; zur Loye, H.-C.; DiPrete, D. P.; Amoroso, J. W.; **Shustova, N. B.*** "Boarding-up": Radiation Damage and Radionuclide

- Leaching Kinetics in Linker-Capped Metal-Organic Frameworks" *Inorg. Chem.* **2020**, *59*, 179–183. (highlighted in "Inorganic Chemistry Forum on "Innovative f-Element Chelating Strategies").
74. Shakya, D. M.; Ejegbavwo, O. A.; Rajeshkumar, T.; Senanayake, S. D.; Brandt, A. J.; Farzandh, S.; Acharya, N.; Ebrahim, A. M.; Frenkel, A. I.; Rui, N.; Tate, G. L.; Monnier, J. R.; Vogiatzis, K. D.; **Shustova, N. B.***; Chen, D. A. "Selective Catalytic Chemistry at Rhodium (II) Nodes in Bimetallic Metal-Organic Frameworks" *Angew. Chem. Int. Ed.* **2019**, *131*, 58, 16533–16537.
 73. Dolgoplova, E. A.; Galitskiy, V. A.; Martin, C. R.; Gregory, H. N.; Yarbrough, B. J.; Rice, A. M.; Berseneva, A. A.; Ejegbavwo, O. A.; Stephenson, K. S.; Kittikhunnatham, P.; Karakalos, S. G.; Smith, M. D.; Greytak, A. B.; Garashchuk, S.; **Shustova, N. B.*** "Connecting Wires: Photoinduced Electronic Structure Modulation in Metal-Organic Frameworks *J. Am. Chem. Soc.*, **2019**, *141*, 5350–5355.
 72. Rice, A. M.; Leith G. A.; Ejegbavwo, O. A.; Dolgoplova, E. A.; **Shustova, N. B.*** "Heterometallic Metal-Organic Frameworks (MOFs): The Advent of Improving the Energy Landscape" *ACS Energy Lett.*, **2019**, *4*, 1938–1946 (highlighted on the cover).
 71. Pandey, S.; Jia, Z.; Demaske, B.; Ejegbavwo, O. A.; Setyawan, W.; Henager, C. H.; Shustova, N. B.; Phillpot, S. R. "Sequestration of Radionuclides in Metal-Organic Frameworks from Density Functional Theory Calculations" *J. Phys. Chem. C* **2019**, *123*, 26842–26855.
 70. Williams, D. E.; Martin, C. R.; Dolgoplova, E. A.; Swifton, A.; Godfrey, D. C.; Ejegbavwo, O. A.; Pellechia, P.; Smith, M. D.; **Shustova, N. B.*** "Flipping the Switch: Fast Photoisomerization in a Confined Environment" *J. Am. Chem. Soc.*, **2018**, *40*, 7611–7622 (highlighted on the cover).
 69. Rice, E. A.; Dolgoplova E. A.; Yarbrough, B. J.; Leith G. A.; Martin C. R.; Stephenson, K. S.; Heugh, R. A.; Brandt, A. J.; Chen, D. A.; Karakalos, S. G.; Smith M. D.; Hatzell, K. B.; Pellechia, P. J.; Garashchuk, S.; Shustova, N. B. "Stack the Bowls: Tailoring the Electronic Structure of Corannulene-Integrated Crystalline Materials" *Angew. Chem. Int. Ed.* **2018**, *57*, 11310–11315.
 68. Dolgoplova, E. A.; Rice, A. M.; **Shustova, N. B.*** "Photochemistry and Photophysics of MOFs: Steps Towards MOF-based Sensing Enhancements" *Chem. Soc. Rev.* **2018**, *47*, 4710–4728 (highlighted on the cover).
 67. Dolgoplova, E. A.; Rice, A. M.; **Shustova, N. B.*** "Actinide-based MOFs: A Middle Ground in Solution and Solid-State Structural Motifs" *Chem. Commun. (Emerging Investigator Issue)* **2018**, *54*, 6472–6483 (highlighted on the cover).
 66. zur Loye, H.-C.; Besmann, T.; Amoroso, J.; Brinkman, K.; Grandjean, A.; Henager, C. H.; Hu, S.; Mixture, S. T.; Phillpot, S. R.; **Shustova, N. B.**; Wang, H.; Koch, R. J.; Morrison, G.; Dolgoplova, E. "Hierarchical Materials as Tailored Nuclear Waste Forms: A Perspective" *Chem. Mater.* **2018**, *30*, 4475–4488.
 65. Baroni, N.; Turshatov, A.; Adams, M.; Dolgoplova, E. A.; Schliiske, S.; Hernandez-Sosa, G.; Wöll, C.; Shustova, N. B.; Richards, B. S.; Howard, I. A. "Inkjet-Printed Photoluminescent Patterns of Aggregation-Induced-Emission Chromophores on Surface-Anchored Metal-Organic Frameworks" *ACS Appl. Mater. Interfaces*, **2018**, *10*, 25754–25762.
 64. Dolgoplova, E. A.; Brandt, A. J.; Ejegbavwo, O. A.; Duke, A. S.; Maddumapatabandi, T. D.; Galhenage, R. P.; Larson, B. W.; Reid, O. G.; Ammal, S. C.; Heyden, A.; Chandrashekhar, M.; Stavila, V.; Chen, D. A.; **Shustova, N. B.*** "Electronic Properties of Bimetallic Metal-Organic Frameworks (MOFs): Tailoring the Density of Electronic States through MOF Modularity" *J. Am. Chem. Soc.*, **2017**, *139*, 5201–5209.
 63. Dolgoplova, E. A.; Ejegbavwo, O. A.; Martin, C. R.; Smith, M. D.; Setyawan, W.; Karakalos S. G.; Henager, C. H.; zur Loye, H.-C.; **Shustova, N. B.*** "Multifaceted Modularity: A Key for Stepwise Building of Hierarchical Complexity in Actinide Metal-Organic Frameworks" *J. Am. Chem. Soc.*, **2017**, *39*, 16852–16861.
 62. Rice, A. M.; Fellows, W. B.; Dolgoplova, E. A.; Greytak, A. B.; Vannucci, A. K.; Smith, M. D.; Karakalos, S. G.; Krause, J. A.; Avdoshenko, S. M.; Popov, A. A.; **Shustova, N. B.*** "Hierarchical Corannulene-Based Materials: Energy Transfer and Solid-State Photophysics" *Angew. Chem. Int. Ed.* **2017**, *56*, 4525–4529.
 61. Rice, A. M.; Dolgoplova, E. A.; **Shustova, N. B.*** "Fulleretic Materials: Buckyball- and Buckybowl-Based Crystalline Frameworks" *Chem. Mater.* **2017**, *29*, 7054–7061.
 60. Dolgoplova, E. A.; Moore, T. C.; Ejegbavwo, O. A.; Pellechia, P.; Smith, M. D.; **Shustova, N. B.*** "A Metal-Organic Framework as a Flask: Photophysics of Confined Chromophores with a Benzyldiene Imidazolinone Core" *Chem. Commun. (Emerging Investigator Issue)*, **2017**, *53*, 7361–7364.
 59. Dolgoplova, E. A.; **Shustova, N. B.*** "Metal-Organic Framework Photophysics: Optoelectronic Devices, Photoswitches, Sensors, and Photocatalysts" *MRS Bulletin*, **2016**, *41*, 890–896 (highlighted on the cover).
 58. Fellows, B. W.; Rice, A. M.; Williams, D. E.; Dolgoplova, E. A.; Vannucci, A. K.; Pellechia, P. J.; Smith, M. D.; Krause, J. A.; **Shustova, N. B.*** "Redox-Active Corannulene Buckybowls in a Crystalline Hybrid Scaffold" *Angew. Chem. Int. Ed.* **2016**, *55*, 2195–2199 (highlighted on the cover).
 57. Williams, D. E.; Godfrey, D. C.; Ermolaeva, E. D. Pellechia, P. J.; Greytak, A. B.; Smith, M. D.; Avdoshenko, S. M.; Popov, A. A.; **Shustova, N. B.*** "Fulleretic Well-Defined Scaffolds: Donor-Fullerene Alignment Through Metal Coordination and Its Effect on Photophysics" *Angew. Chem. Int. Ed.* **2016**, *55*, 9070–9074.

56. Dolgoplova, E. A.; Rice, A. M.; Smith, M. D.; **Shustova, N. B.** "Photophysics, Dynamics, and Energy Transfer in Rigid Mimics of GFP-based Systems" *Inorg. Chem.* **2016**, *55*, 7257–7264.
55. Dolgoplova, E. A.; Moore, T. M.; Fellows, W. B.; Smith, M. D.; **Shustova, N. B.** "Photophysics of GFP-related Chromophores Imposed by a Scaffold Design", *Dalton Trans. (New Talents: Americas)*, **2016**, 45, 9884–9891.
54. Dolgoplova, E. A.; Williams, D. E.; Greytak, A. B.; Rice, A. M.; Smith, M. D.; Krause, J. A.; **Shustova, N. B.** "A Bio-inspired Approach for Chromophore Communication: Ligand-to-Ligand and Host-to-Guest Energy Transfer in Hybrid Crystalline Scaffolds" *Angew. Chem. Int. Ed.* **2015**, *54*, 13639–13643.
53. Williams, D. E.; Dolgoplova, E. A.; Pellechia, P. J.; Palukoshka, A.; Wilson, T. J.; Tan, R.; Maier, J. M.; Tan, R.; Greytak, A. B.; Smith, M. D.; Krause, J. A.; **Shustova, N. B.** "A Mimic of the Green Fluorescent Protein β -barrel: Photophysics and Dynamics of Confined Chromophores Defined by a Rigid Porous Scaffold" *J. Am. Chem. Soc.* **2015**, *137*, 2223–2226.
52. Duke, A. S.; Dolgoplova, E. A.; Galhenage, R. P.; Ammal, S. C.; Heyden, A.; Smith, M. D.; Chen, D. A.*; **Shustova, N. B.** "Active Sites in Copper-based Metal-Organic Frameworks: Understanding Substrate Dynamics, Redox Processes, and Valence-Band Structure" *J. Phys. Chem. C* **2015**, *119*, 27457–27466.
51. Williams, D. E.; **Shustova, N. B.** "Metal-Organic Frameworks as a Versatile Tool to Study and Model Energy Transfer Processes" *Chem. Eur. J.* **2015**, *21*, 15474–15479.
50. Gardinier, J. R.*; Hewage, J. S.; Justin Hoffman, Lindeman, S. V.; Williams, D. E.; **Shustova, N. B.** "Supramolecular Assembly of Metal-Organic Tubes Constructed from the Ditopic Heteroscorpionate Ligand (4-NH₂C₆H₄)CHpz₂ (pz = Pyrazol-1-yl) and Silver(I)" *Eur. J. Inorg. Chem.* **2016**, 2615–2625.
49. Williams, D. E.; Rietman, J. A.; Maier, J. M.; Tan, R.; Greytak, A. B.; Smith, M. D.; Krause, J. A.; **Shustova, N. B.** "Energy Transfer on Demand: Photoswitch-Directed Behavior of Metal-Porphyrin Frameworks" *J. Am. Chem. Soc.* **2014**, *136*, 11886–11889.
48. Boltalina, O. V.; Kuvychko, I. V.; Popov, A. A.; **Shustova, N. B.**; Strauss, S. H. "Perfluoroalkylfullerenes" *Chem. Rev.* **2015**, *115*, 1051–1105.
47. Whitaker, J. B.; Kuvychko, I. V.; **Shustova, N. B.**; Chen, Y.-S.; Strauss, S. H. Boltalina, O. V. "An elusive fulvene 1,7,11,24-C₆₀(CF₃)₄ and its unusual reactivity" *Chem. Commun.* **2014**, *50*, 1205–1208.
46. **Shustova, N. B.**; Cozzolino, A. F.; Reineke, S.; Baldo, M.; Dincă, M. "Selective Turn-On Ammonia Sensing Enabled by High-Temperature Fluorescence in Metal–Organic Frameworks with Open Metal Sites" *J. Am. Chem. Soc.* **2013**, *135*, 13326–13329.
45. Clikeman, T. T.; Kuvychko, I. V.; **Shustova, N. B.**; Chen, Y.-S.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "Regioselective Sequential Additions of Nucleophiles and Electrophiles to Perfluoroalkylfullerenes: Which Cage C Atoms Are the Most Reactive and Why?" *Chem. Eur. J.* **2013**, *19*, 5070–5080.
44. Whitaker, J. B.; **Shustova, N. B.**; Strauss, S. H.; Boltalina, O. V. "Structure of 7,9,12,15,18,20,39,24,45,57-C₆₀(CF₃)₁₀(1,2:3,4-O₂) The First Regiospecific Diepoxidation of a Fullerene Derivative" *Acta Chim. Slov.* **2013**, *60*, 577–582 (a special issue in honor of Prof. Žemva).
43. **Shustova, N. B.**; Ong, T.-C.; Cozzolino, A. F.; Michaelis, V. K.; Griffin, R. G.; Dincă, M. "Phenyl Ring Dynamics in a Tetraphenylethylene-Bridged Metal-Organic Framework: Implications for the Mechanism of Aggregation-Induced Emission" *J. Am. Chem. Soc.* **2012**, *134*, 15061–15070.
42. **Shustova, N. B.**; Cozzolino, A. F.; Dincă, M. "High-Energy Conformational Locking and Fluorescence in an Ethynyl-Extended Tetraphenylethylene-Based Metal-Organic Framework" *J. Am. Chem. Soc.* **2012**, *134*, 19596–19599.
41. **Shustova, N. B.**; McCarthy, B. D.; Dincă, M. "Turn-On Fluorescence in Tetraphenylethylene-Based Metal-Organic Frameworks: an Alternative to Aggregation-Induced Emission" *J. Am. Chem. Soc.* **2011**, *133*, 20126–20129.
40. **Shustova, N. B.**; Peryshkov, D. V.; Kuvychko, I. V.; Chen, Y.-S.; Mackey, M. A.; Coumbe, C. E.; Heaps, D. T.; Confait, B. S.; Heine, T.; Phillips, J. P.; Stevenson, S.; Dunsch, L.; Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "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*, 2672–2690.
39. **Shustova, N. B.**; Kuvychko, I. V.; Popov, A. A.; Delius, M.; Dunsch, L.; Anderson, O. P.; Hirsch, A.; Strauss, S. H.; Boltalina, O. V. "Nitrogen Directs Multiple Radical Additions to 9,9'-Bi-1-aza(C₆₀-I_h)[5,6]fullerene. X-ray Structure of 6,9,12,15,18-C₅₉N(CF₃)₅" *Angew. Chem. Int. Ed.* **2011**, 5537–5540.
38. **Shustova, N. B.**; Kuvychko, I. V.; Peryshkov, D. V.; Whitaker, J. B.; Larson, B. W.; Chen, Y.-S.; Dunsch, L.; Seppelt, K.; Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "Chemical Tailoring of Fullerene Acceptors: Synthesis, Structures and Electrochemical Properties of Perfluoroisopropylfullerenes" *Chem. Commun.* **2011**, 47, 875–877.
37. Kuvychko, I. V.; Whitaker, J. B.; Larson, B. W.; Folsom, T. C.; **Shustova, N. B.**; Avdoshenko, S. M.; Chen, Y.-S.; Wen, H.; Wang, X. B.; Dunsch, L.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "Substituent Effects in a Series of 1,7-C₆₀(R-F)₂

- Compounds (R-F = CF₃, C₂F₅, *n*-C₃F₇, *i*-C₃F₇, *n*-C₄F₉, *s*-C₄F₉, *n*-C₈F₁₇): Electron Affinities, Reduction Potentials and E(LUMO) Values Are Not Always Correlated" *Chem. Sci.* **2012**, 3, 1399–1407.
36. Kuvychko, I. V.; **Shustova, N. B.**; Avdoshenko, S. M.; Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "In Search of Fullerene-Based Superacids: Synthesis, X-ray Structure, and DFT study of C₆₀(C₂F₅)H" *Chem. Eur. J.*, **2011**, 17, 8799–8802.
 35. **Shustova, N. B.**; Mazej, Z.; Chen, Y.-S.; Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "Saturnene Revealed : X-ray Crystal Structure of D_{5d}-C₆₀F₂₀ Formed in Reactions of C₆₀ with A_xMF_y Fluorinating Agents (A = Alkali Metal ; M = 3d Metal)" *Angew. Chem. Int. Ed.* **2010**, 49, 812–815.
 34. **Shustova, N. B.**; Kareev, I. E.; Kuvychko, I. V.; Whitaker, J. B.; Lebedkin, S. F.; Popov, A. A.; Dunsch, L.; Chen, Y.-S.; Seppelt, K.; Strauss, S. H.; Boltalina, O. V. "High-temperature and photochemical syntheses of C₆₀ and C₇₀ fullerene derivatives with linear perfluoroalkyl chains" *J. Fluorine Chem.* **2010**, 131, 1198–1212.
 33. Kuvychko, I. V.; Streletskii, A. V.; **Shustova, N. B.**; Seppelt, K.; Drewello, Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "Soluble Chlorofullerenes C₆₀Cl_{2,4,6,8,10}. Synthesis, Purification, Compositional Analysis, Stability, and Experimental/Theoretical Structure Elucidation, Including the X-ray Structure of C₁-C₆₀Cl₁₀" *J. Am. Chem. Soc.* **2010**, 132, 6443–6462.
 32. Popov, A. A.; **Shustova, N. B.**; Svitova, A. L.; Mackey, M. A.; Coumbe, C. E.; Phillips, J. P.; Stevenson, S.; Strauss, S. H.; Boltalina, O. V.; Dunsch, L. "Redox-Tuning Endohedral Fullerene Spin States: From the Dication to the Trianion Radical of Sc₃N@C₈₀(CF₃)₂ in Five Reversible Single-Electron Steps" *Chem.-Eur. J.* **2010**, 16, 4721–4724.
 31. Popov, A. A.; Kareev, I. E.; **Shustova, N. B.**; Strauss, S. H.; Boltalina, O. V.; Dunsch, L. "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 C₆₀(CF₃)_{2n} (2n = 2–10) Derivatives and Density Functional Theory-Assisted Assignment" *J. Am. Chem. Soc.* **2010**, 132, 1709–11721.
 30. **Shustova, N. B.**; Chen, Y.-S.; Mackey, M. A.; Coumbe, C. E.; Phillips, J. P.; Stevenson, S.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "Sc₃N@C₈₀-I_h(7)(CF₃)₁₄ and Sc₃N@C₈₀-I_h(7)(CF₃)₁₆. Endohedral Metallofullerene Derivatives with Exohedral Addends on Four and Eight Triple-Hexagon Junctions. Does the Sc₃N Cluster Control the Addition Pattern or Vice Versa?" *J. Am. Chem. Soc.* **2009**, 131, 17630–17637.
 29. Kareev, I. E.; Kuvychko, I. V.; **Shustova, N. B.**; Lebedkin, S. F.; Bubnov, V. P.; Anderson, O. P.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "C₁-(C₈₄-C₂(11))(CF₃)₁₂ : Trifluoromethylation Yields Structural Proof of a Minor C₈₄ Cage and Reveals a Principle of Higher Fullerene Reactivity" *Angew. Chem. Int. Ed.* **2008**, 120, 6204–6207.
 28. Kareev, I. E.; Popov, A. A.; Kuvychko, I. V.; **Shustova, N. B.**; Lebedkin, S. F.; Bubnov, V. P.; Anderson, O. P.; Seppelt, K.; Strauss, S. H.; Boltalina, O. V. "Synthesis and X-ray or NMR/DFT structure elucidation of twenty-one new trifluoromethyl derivatives of soluble cage isomers of C₇₆, C₇₈, C₈₄, and C₉₀" *J. Am. Chem. Soc.* **2008**, 130, 13471–13489.
 27. **Shustova, N. B.**; Serov, M.; Troyanov, S. I. "Molecular and crystal structure of the C₆₀F₁₈ adducts with bromine and carbon disulfide" *Fullerenes Nanotubes Carbon Nanosruct.* **2008**, 16, 597–602.
 26. **Shustova, N. B.**; Kuvychko, I. V.; Boltalina, O. V.; Strauss, S. H. "1,7,16,30,36,47-Hexakis(perfluoroisopropyl)-1,7,16,30,36,47-hexahydro(C₆₀-I_h)[5,6]fullerene" *Acta Cryst.* **2007**, E63, o4575.
 25. Popov, A. A.; **Shustova, N. B.**; Boltalina, O. V.; Strauss, S. H.; Dunsch, L. "ESR-Vis-NIR Spectroelectrochemical Study of C₇₀(CF₃)₂²⁻ and C₇₀(C₂F₅)₂²⁻ Radical Anions" *ChemPhysChem* **2008**, 9, 431–438.
 24. Popov, A. A.; Kareev, I. E.; **Shustova, N. B.**; Lebedkin, S. F.; Strauss, S. H.; Boltalina, O. V.; Dunsch, L. "Synthesis, Spectroscopic and Electrochemical Characterization, and DFT Study of Seventeen C₇₀(CF₃)_n Derivatives (n=2, 4, 6, 8, 10, 12)" *Chem. Eur. J.* **2008**, 14, 107–121.
 23. **Shustova, N. B.**; Anderson, O. P.; Boltalina, O. V.; Strauss, S. H. "1,3,7,10,14,17,21,28,31,42,52,55-Dodecakis(trifluoromethyl)-1,3,7,10,14,17,21,28,31,42,52,55-dodecahydro(C₆₀-I_h)[5,6]fullerene" *Acta Cryst.* **2007**, E64, o159.
 22. **Shustova, N. B.**; Popov, A. A.; Mackay, M. A.; Coumbe, C. E.; Phillips, J. P.; Stevenson, S.; Strauss, S. H.; Boltalina, O. V. "Radical Trifluoromethylation of Sc₃N@C₈₀" *J. Am. Chem. Soc.* **2007**, 129, 11676–11677.
 21. **Shustova, N. B.**; Kuvychko, I. V.; Bolskar, R. D.; Seppelt, K.; Strauss, S. H.; Boltalina, O. V. "Trifluoromethyl Derivatives of Insoluble Small-HOMO-LUMO-Gap Hollow Higher Fullerenes. NMR and DFT Structure Elucidation of C₂-(C₇₄-D_{3h})(CF₃)₁₂, C_s-(C₇₆-T_d)(CF₃)₁₂, C₂-(C₇₈-D_{3h}(5))(CF₃)₁₂, C_s-(C₈₀-C_{2v}(5))(CF₃)₁₂, and C₂-(C₈₂-C₂(5))(CF₃)₁₂" *J. Am. Chem. Soc.* **2006**, 128, 15793–15798.
 20. **Shustova, N. B.**; Newell, B. S.; Miller, S. M.; Anderson, O. P.; Bolskar, R. D.; Seppelt, K.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "Discovering and Verifying Fullerene Cage Isomers: Structures of C₂-p¹¹-(C₇₄-D_{3h})(CF₃)₁₂ and C₂-p¹¹-(C₇₈-D_{3h}(5))(CF₃)₁₂" *Angew. Chem. Int. Ed.* **2007**, 46, 4111–4114.
 19. Popov, A. A.; Kareev, I. E.; **Shustova, N. B.**; Stukalin, E. B.; Lebedkin, S. F.; Seppelt, K.; Strauss, S. H.; Boltalina, O. V.; Dunsch, L. "Electrochemical, Spectroscopic, and DFT Study of C₆₀(CF₃)_n Frontier Orbitals (n = 2–18): The Link between Double Bonds in Pentagons and Reduction Potentials" *J. Am. Chem. Soc.* **2007**, 129, 11551–11568.

18. Kareev, I. E.; **Shustova, N. B.**; Kuvychko, I. V.; Lebedkin, S. F.; Miller, S. M.; Anderson, O. P.; Popov, A. A.; Strauss, S. H.; Boltalina, O. V. "Thermally-Stable Perfluoroalkylfullerenes With the Skew-Pentagonal Pyramid Pattern: $C_{60}(C_2F_5)_4O$, $C_{60}(CF_3)_4O$, and $C_{60}(CF_3)_6$ " *J. Am. Chem. Soc.* **2006**, *128*, 12268–12280.
17. **Shustova, N. B.**; Peryshkov, D. V.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "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.* **2007**, *E63*, o3129.
16. **Shustova, N. B.**; Peryshkov, D. V.; Kareev, I. E.; Boltalina, O. V.; Strauss, S. H. "1,6,11,18,24,27,33,51,54,60-Octakis(trifluoromethyl)-1,6,11,18,24,27,33,51,54,60-octahydro($C_{60}-I_h$)[5,6]fullerene deuteriochloroform solvate" *Acta Cryst.* **2007**, *E63*, o3398.
15. **Shustova, N. B.**; Peryshkov, D. V.; Kareev, I. E.; Boltalina, O. V.; Strauss, S. H. "1,4,7,11,18,21,24,31,35,39,51,58,61,64-Tetradecakis(trifluoromethyl)-1,4,7,11,18,21,24,31,35,39,51,58,61,64-tetradecahydro($C_{70}-D_{5h}$)[5,6]fullerene p-xylene trisolvate" *Acta Cryst.* **2007**, *E63*, o3928–o3929.
14. Kareev, I. E.; **Shustova, N. B.**; Peryshkov, D. V.; Lebedkin, S. F.; Miller, S. M.; Anderson, O. P.; Popov, A. A.; Boltalina, O. V.; Strauss, S. H. "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**, 1650–1652.
13. **Shustova, N. B.**; Peryshkov, D. V.; Boltalina, O. V.; Strauss, S. H. "1,4,10,19,25,41,55,60,67,69-Decakis(trifluoromethyl)-1,4,10,19,25,41,55,60,67,69-decahydro($C_{70}-D_{5h}$)[5,6]fullerene" *Acta Cryst.* **2007**, *E63*, o4073.
12. Kareev, I. E.; **Shustova, N. B.**; Newell, B. S.; Miller, S. M.; Anderson, O. P.; Strauss, S. H.; Boltalina, O. V. "1,6,11,18,24,27,52,55-Octakis(trifluoromethyl)-1,6,11,18,24,27,52,55-octahydro($C_{60}-I_h$)[5,6]fullerene" *Acta Cryst.* **2006**, *E62*, o3154–o3156.
11. Troyanov, S.; **Shustova, N.**; Popov, A.; Ioffe, I.; Kemnitz, E. "Structure of Halofullerenes Using Experimental and Theoretical Approaches" *Acta Cryst.* **2005**, *A61*, 19–20.
10. **Shustova, N. B.**; Chernyshev, D. Y.; Troyanov S. I. "Crystal Structure C_{60} Prepared by a Reaction C_{60} with $POCl_3$ " *Mendeleev Commun.* **2006**, *4*, 209–210.
9. Troyanov, S. I.; **Shustova, N. B.**; Popov, A. A.; Sidorov, L. N.; Kemnitz, E. "Preparation and Structural Characterization of Two Kinetically Stable Chlorofullerenes, $C_{60}Cl_{28}$ and $C_{60}Cl_{30}$ " *Angew. Chem. Int. Ed.* **2005**, *44*, 432–435.
8. **Shustova, N. B.**; Popov, A. A.; Sidorov, L. N.; Turnbull, A. P.; Kemnitz, E.; Troyanov, S. I. "Preparation and Crystallographic Characterization of $C_{60}Cl_{24}$ " *Chem. Commun.* **2005**, 1411–1413.
7. Troshin, P. A.; Lyubovskaya, R. N.; Ioffe, I. N.; **Shustova, N. B.**; Kemnitz, E.; Troyanov, S. I. "Synthesis and Structure of the Highly Chlorinated [60]fullerene $C_{60}Cl_{30}$ with a Drum-Shaped Carbon Cage" *Angew. Chem. Int. Ed.* **2005**, *44*, 234–237.
6. Troyanov, S. I.; **Shustova, N. B.**; Ioffe, I. N.; Turnbull, A. P.; Kemnitz, E. "Synthesis and Structural Characterization of Highly Chlorinated C_{70} , $C_{70}Cl_{28}$ " *Chem. Commun.* **2005**, 72–74.
5. Troyanov, S. I.; **Shustova, N. B.**; Popov, A. A.; Sidorov, L.N. "Synthesis and Structure of C_{60} Fullerene Chlorides" *Russ. Chem. Bull.* **2005**, *54*, 1656–1666.
4. Sidorov, L. N.; Livadaris, V.; **Shustova, N. B.**; Ioffe, I. N.; Kemnitz, E.; Troyanov, S. I. "Electron Affinity and Suppression Effect in Analysis of Chlorofullerenes by MALDI Mass Spectrometry" *Russ. Chem. Bull.* **2005**, *54*, 1121–1124.
3. Troyanov, S. I.; **Shustova, N. B.**; Popov, A. A.; Feist, M.; Kemnitz, E. "Synthesis and Properties of Inorganic Compounds Fullerene C_{60} and C_{70} Chlorination using Chlorides $SbCl_5$ and VCl_4 " *Russ. J. Inorg. Chem.* **2004**, *49*, 1303–1307.
2. Alyoshina V. E., Borshchevsky A. Ya., Dorozhkin E. I., Goryunkov A. A., Astakhov A. V., **Shustova N. B.**, Ovchinnikova N. S. "Negative Ions of Trifluoromethyl Fullerene Derivatives: First Thermodynamic data" *Fullerenes, Nanotubes, and Carbon Nanostruct.* **2004**, *12*, 201–207.
1. Aleshina, V. E.; Borschevskii, A. Ya.; Skokan, E. V.; Arhangelskii, I. V.; Astahov, A. V.; **Shustova, N. B.** "Fluorination of the Cubic and Hexagonal C_{60} Modifications by Crystalline Manganese Trifluoride" *Phys. Solid State* **2002**, *44*, 629–630.

Selected Invited Talks

MIT-Harvard; University of California, Berkeley; University of Chicago; Northwestern University; Imperial College, London; ETH Zurich; Cornell University; University of Pennsylvania; Texas A&M University, University of Utah, University of South California, Boston College, University of California, Riverside; University of Colorado, Boulder; University of Pittsburgh; Vanderbilt University, Colorado State University, Emory University; Marquette University, Florida State University, Georgia Institute of Technology; Dartmouth College; Brandies University, University of North Carolina, Chapel Hill; University of Iowa; Gordon Conferences (2017–2024); MOF (2016, 2018, 2022, 2024); euro-MOF (2019); ICCG (2018, 2024).

Awarded Research Support

DOE, Catalysis	2022–2026
NSF, DMR	2025–2028
NSF, DMR	2024–2025
DOE, Catalysis	2021–2026
NSF, DMR	2021–2026

DOE, Catalysis	2021–2022
IAS Hans Fisher Fellowship	2021–2024
DOE EFRC – Center for Hierarchical Waste Form Materials (leading PI)	2020–2024
NSF EPSCOR GEAR	2021–2023
Camille Dreyfus Teaching Scholar Award	2019–2024
NSF CAREER – Division of Materials Research, Solid State and Materials Chemistry	2016–2022
E-conversion Cluster Grant	2021–2024
USC ASPIRE-II Research Grant	2020–2023
McCausland Fellowship	2019–2022
NASA	2020–2021
DOE EFRC – Center for Hierarchical Waste Form Materials (leading PI)	2017–2020
DOE, Catalysis	2018–2021
USC ASPIRE-II Research Grant	2018–2019
Cottrell Scholar Research Grant	2017–2019
Alfred P. Sloan Research Fellowship	2017–2019
DOE/Savannah River National Laboratory	2018–2019
SC EPSCoR-SAN/SC	2018–2019
Savannah River National Laboratory/DOE	2016–2017
ACS PRF	2014–2016
USC ASPIRE-III Research Grant	2014–2015
USC ASPIRE-I Research Grant	2014–2015
EPSCoR IDeA NSF	2015

Service and Outreach

International Organization Advisory Committee	2022–present
Associate Editor of <i>ACS Materials Letters</i>	2022–present
Executive Committee for the Beckman Foundation	2023–present
ACS Award Selection and Nomination Committee	2019–2022
Research Corporation Science and Advancement, Cottrell Selection Committee	2022–present
Associate Editor of <i>Materials Frontiers</i>	2016–2019
Chair and Chair of Elect of the ACS Inorganic Subdivision	2020, 2021
Director of Women-in-Science (Wi-Sci) Educational Program for Carolinas	2013–present
University Senate	2019–2022
Editorial Board Member of <i>ACS Applied Materials & Interfaces</i>	2019–present
Industrial & Engineering Chemistry Research, Reviews and Advances in Chemistry (ReACh)	2019–present
Organizer ACS Inorganic Chemistry Series	2020
Conference and Symposium Organizer: International Pacific Chem (2021), International NanoGe (2022), ACS SERMACs (2016, 2019), and National NC Photochem (2018–2023)	
Active Participant of Undergraduates from the SC-AMP Outreach Research Program for High School Students from the SPRI Summer Research Program	2015–present
University Fulbright Committee for Undergraduate Students	2019–present
External Thesis Committee for the Following Countries: Australia, Germany, and India	2015–present
External Reviewers for the Following Countries (besides USA): Germany, Belgium, Cyprus, and China	2021–present
Undergraduate Research Advisor (more than 50 undergraduates)	2013–present
Department of Chemistry Admission Committee	2013–2019
Freshman Advisor	2014–2023
Departmental Executive Committee	2023–present
Departmental Award Committee	2023–present
Bouknight Scholarship Award Committee	2023–present
Departmental Safety Committee	2018–present
Departmental Seminar Committee	2023–present
Reviewer for Science, Nature Publishing Group, ACS, RSC, and Wiley-VCH journals	2013–present

Teaching Experience

CHEM 111	<i>General Chemistry</i> (Fall 2014, Spring 2015, Fall 2016, Spring 2016, Fall 2017, Spring 2018, Fall 2022, Fall 2023, Fall, 2024, Fall 2025). Introductory Chemistry Course for ~200–300 students
CHEM 711	<i>Physical Methods in Inorganic Chemistry</i> (Spring 2019, 2020; Fall 2021, Spring 2022, 2024, 2025) Principles of Group Theory as Applied to Electronic Structure in Inorganic Chemistry and Spectroscopy
CHEM 719	<i>Materials for Renewable Energy Applications</i> (Fall 2013, Fall 2017) Introduction to fundamental concepts of energy conversion: photovoltaics, light-emitting diodes, thermoelectric materials, alternative fuels, electrochemical energy storage, and batteries and capacitors.
CHEM 713	<i>Chemistry of Representative Elements</i> (Fall 2019, Fall 2020)