

Curriculum Vitae

Radu Custelcean

Senior Research Scientist, Oak Ridge National Laboratory

Chemical Separations Group, Chemical Sciences Division, Oak Ridge National Laboratory, PO Box 2008, MS 6119, Oak Ridge, TN 37831-6119; Tel: (865) 574-5018; (612) 382-4799 (cell)
E-mail: custelceanr@ornl.gov

Web of Science ResearcherID: <http://www.researcherid.com/rid/C-1037-2009>

Google Scholar: https://scholar.google.com/citations?user=_Ofy4OEAAA&hl=en
orcid.org/0000-0002-0727-7972

Education

2000 Ph.D. Organic Chemistry, Michigan State University

Thesis: *"Topochemical Assembly of Covalent Materials using Dihydrogen Bonds"*

1996 M.S. Organic Chemistry, Babeş-Bolyai University, Romania

1995 B.S. Chemistry, Babeş-Bolyai University, Romania

Professional Experience

2020-present Senior Research Scientist, Oak Ridge National Laboratory

2008-2019 Research Scientist, Oak Ridge National Laboratory

2003-2008 R&D Associate, Oak Ridge National Laboratory
crystalline materials for energy and environmental applications; supramolecular chemistry; crystal engineering; chemical separations; anion recognition; carbon capture; structural chemistry; X-ray crystallography

2002-2003 Senior Research Associate, Institute for Shock Physics, Washington State University

energetic materials; materials under extreme pressures; Raman spectroscopy

2000-2002 Postdoctoral Associate, Dept. of Chem. Eng. and Materials Science, University of Minnesota

crystal engineering; solid-state organic chemistry; hydrogen-bonded materials

Research Interests: separation science and technology; supramolecular chemistry; crystal engineering; self-assembled materials for energy and environmental applications; anion recognition; CO₂ capture; X-ray crystallography.

Recognitions, Honors, Awards

- 2021 R&D100 Award for BIG NET Technology

- ORNL Innovation Awards, 2020, 2021

- *Margaret Etter* Early Career Award from the *American Crystallographic Association*, 2008

- Finalist (Top 3), Early Career Award for Scientific Accomplishment, UT-Battelle, 2005

- *Harold Hart* Endowed Fellowship, Michigan State University, 2000

- Third place, National Chemistry Olympiad (Romania 1990)

- 19 papers featured on journal covers: *JACS Au* (2023), *ACS Applied Materials & Interfaces* (2023), *MRS Bulletin* (2022) *Cell Reports Physical Science* (2021), *Chem. Eur. J.* (2022, 2020, 2016), *I&EC Research* (2019) *Angew. Chem.* (2015, 2005), *Chem. Comm.* (2019, 2019, 2013,

2012, 2005), *Cryst. Growth Des.* (2009, 2008), *Eur. J. Inorg. Chem.* (2007), *Struct. Chem.* (1999).

- *Cell Reports Physical Science* paper highlighted in *C&EN News* (2021)
- *ChemSusChem* paper *Dialing in Direct Air Capture of CO₂ by Crystal Engineering of Bis-aminoguanidines* highlighted in the *ChemViews* magazine (2020)
- *Chem* paper “CO₂ Capture via Crystalline Hydrogen-Bonded Bicarbonate Dimers” was selected to the Best of Chem 2019 special reprint collection.
- *Chem* paper on CO₂ capture highlighted in *Science*, *Phys.org*, *New Scientist*, and more than a dozen other news outlets. Featured as a Science Headline on the DOE’s Office of Science website (2019).
- interview with the WTOP radio station (Washington D.C. area) about our direct air capture of CO₂ technology (2018)
- *Nature Energy* paper on direct air capture of CO₂ highlighted on the DOE Office of Science homepage as a science headline, and selected as one of the top 5 stories for 2018 from the Office of Science. The press release was picked up by several news outlets, including Knoxville News Sentinel, Oak Ridger, Yahoo News, Digital Trends, TechXplore, Science and Technology Research News. The news was also tweeted by DOE and Battelle (2018).
- *Angew. Chem.* paper on CO₂ capture from air highlighted on the DOE Office of Science homepage and picked up by several news outlets, including *Phys.org*, Knoxville News Sentinel, Yahoo News, *Materials Today*, *Forbes*, and *USA Today* (2017).
- *Angew. Chem.* paper on self-assembled cage receptor highlighted in *Chemistry World* (2009)
- *ChemComm* paper on sulfate encapsulation highlighted on the ACS webpage (2006)

Professional Activities

- 2023-present, Associate Editor, *Frontiers in Energy Research – Carbon Capture, Utilization and Storage*
- 2022, Guest Editor, *MRS Bulletin Special Issue: Materials for Carbon Capture Technologies*
- Member of the editorial board, *Crystals*, 2020-present
- Member of the editorial board, *Journal of Crystallography*, 2012-2017
- Discussion leader, GRC on Chemical Separations, Galveston, TX, 2020
- Discussion leader, Gordon Research Conference on Crystal Engineering, Stowe, VT, 2016
- Organizer *Climate Change Mitigation Technologies* symposium, MRS Fall 2021
- Organizer *Anion Recognition Chemistry* symposium, PacifiChem 2021
- Organizer *Anion Receptors* symposium, PacifiChem 2015, Honolulu, Hawaii, 2015
- Organizer *Self-Assembled Coordination Architectures* symposium, American Chemical Society meeting, San Francisco, 2014
- Organizer *Self-Assembled Molecular Containers* symposium, American Chemical Society meeting, San Francisco, 2010
- Organizer *Microporous Metal-Organic Framework Solids* symposium, American Crystallographic Association meeting, Orlando FL, 2005

Teaching and Mentoring

2003-present: supervised and mentored 6 postdocs, 2 Ph.D. students, 10 M.S. students, and 5 B.S. students

1996-2000 Teaching Assistant, Department of Chemistry, Michigan State University

- General Chemistry for non-chemistry majors, problem-solving sessions

- Introductory Organic Chemistry for non-chemistry majors, problem-solving sessions
- Organic Chemistry for chemistry majors, problem-solving sessions
- Organic Chemistry laboratory for non-chemistry majors
- Organic Chemistry laboratory for chemistry majors
- Advanced Organic Chemistry (graduate course), lectures and problem-solving sessions

Funding

External

DOE-NAWI, 02/2022–01/2025; *Selective Separation of Selenium Oxyanions by Chelating Hydrogen-Bonding Ligands*, lead PI (with Georgia Tech, Reactwell and TVA) \$1,500,000.

DOE-BES, 09/2021–08/2024; *Interfacial and Photochemical Control of CO₂ Binding, Transport, and Release in Direct Air Capture*, co-PI, \$3,600,000.

TCF Phase 2, DOE Office of Technology Transitions & Office of Fossil Energy, 10/2020–9/2023; *Integrated Process for Direct Air Capture of CO₂ and its Electrochemical Conversion to Ethanol*, lead PI (with Costas Tsouris, Kashif Nawaz, co-PIs), \$1,500,000.

Cooperative Research and Development Agreement (CRADA) with RTM, Germany, 10/2019–9/2021; *Direct Air Capture of CO₂*, lead PI, \$780,000.

DOE-BES, 10/2019–9/2022; *Principles of Chemical Recognition and Transport in Extractive Separations*, lead PI (with Bruce Moyer, Vyacheslav Bryantsev, Santa Jansone-Popova, co-PIs), \$4,900,000.

TCF Phase 1, DOE Office of Technology Transitions & Office of Fossil Energy, 10/2017–12/2018; *Carbon Capture via Crystallization with a Guanidine Ligand*, lead PI, \$300,000 (including \$150,000 ORNL match-up fund).

DOE-BES, 10/2016–9/2019; *Principles of Chemical Recognition and Transport in Extractive Separations*, co-PI (with Bruce Moyer – lead PI, Vyacheslav Bryantsev, Santa Jansone-Popova, Ross Elis co-PIs), \$4,200,000.

DOE-BES, 10/2013–9/2016; *Principles of Chemical Recognition and Transport in Extractive Separations*, co-PI (with Bruce Moyer – lead PI, Benjamin Hay, Laetitia Delmau, Peter Bonnesen co-PIs), \$3,866,000.

DOE-BES Early Career Proposal, *Carbon Capture with Dynamic Covalent Frameworks*, lead PI; awarded \$200,000 for 10/2011-9/2013

DOE-BES Early Career Proposal, *Hierarchical Self-Assembly of Dynamic Covalent Materials with Controlled Architectures and Functionality*, lead PI; awarded \$200,000 for 10/2010-9/2012

DOE-BES, 10/2010–9/2013; *Principles of Chemical Recognition and Transport in Extractive Separations*, co-PI (with Bruce Moyer – lead PI, Benjamin Hay, Laetitia Delmau, Peter Bonnesen co-PIs), \$4,082,000.

DOE-BES, 10/2007–9/2010; *Principles of Chemical Recognition and Transport in Extractive Separations*, co-PI (with Bruce Moyer – lead PI, Benjamin Hay, Laetitia Delmau, Peter Bonnesen co-PIs), \$3,674,000.

DOE-BES, 10/2004–9/2007; *Principles of Chemical Recognition and Transport in Extractive Separations*, co-PI (with Bruce Moyer – lead PI, Benjamin Hay, Laetitia Delmau, Peter Bonnesen co-PIs), \$4,059,000.

Internal

LDRD–ORNL, 10/2021–09/2023; *Direct Air Capture with Aqueous Amino Acids*, lead PI, \$480,000

LDRD-Seed, 4/2021–9/2021; *Photochemically-Driven CO₂ Release in Direct Air Capture*, co-PI (with Yingzhong Ma, lead PI), \$150,000.

LDRD-Seed, 4/2021–9/2021; *Dynamic Ligand Libraries from Direct CO₂ Capture*, co-PI (with Benjamin Doughty, lead PI), \$150,000.

LDRD-Seed, 6/2019–09/2020; *Efficient Process-Intensification Approach for CO₂ Absorption using Amino-Acid Solutions with a Guanidine Compound*, co-PI (with Costas Tsouris, lead PI), \$190,000.

LDRD–ORNL, 10/2011–09/2013; *Novel Covalent Organic Frameworks with Tailored Carbon Capture Functionality*, lead PI (with De-en Jiang, Michelle Kidder, Eduard Hagaman, Sheng Dai co-PIs), \$678,000.

LDRD–ORNL, 10/2009–09/2011; *Controlled Hierarchical Self-Assembly of Robust Organic Architectures*, co-PI (with Benjamin Hay, lead PI), \$600,000.

LDRD-ORNL, 10/2007–09/2009; *Smart Materials Toward a New Paradigm of Super-Efficient Separations Using only Energy Input: Conformational Switching Based on Magnetic Nanoparticles*, co-PI (with Bruce Moyer, lead PI, Peter Bonnesen, Laetitia Delmau, Adam Rondinone, Volker Urban, co-PIs), \$700,000.

Seed Money Fund–ORNL, 10/2008–09/2009; *Ordered Hyperadsorptive Preconcentrators of Threat Agents*, co-PI (with Jun Xu, lead PI), \$175,000.

Publications:

133. Kasturi, A.; Jang, G. G.; Akin, A. D.-T.; Jackson, A.; Jun, J.; Stamberg, D.; Custelcean, R.; Sholl, D. S.; Yiacoumi, S.; Tsouris, C. An Effective Air-Liquid Contactor for CO₂ Direct Air Capture Using Aqueous Solvents. *Separation and Purification Technology* **2023**, *311*, 124398.
132. Hwang, I.; Huang, S.-Y.; Smith, S.; Lynch, V.; Custelcean, R.; Moyer, B. A.; Kumar, N.; Bryantsev, V. S.; Sessler, J. L. Direct Extraction of Sodium Hydroxide by Calix[4]pyrrole-

- Based Ion-Pair Receptors. *J. Am. Chem. Soc.* **2023**, 145, 14387-14394.
131. Premadasa, U. I.; Dong, D.; Stamberg, D.; Custelcean, R.; Roy, S.; Ma, Y.-Z.; Bocharova, V.; Bryantsev, V. S.; Doughty, B. Chemical Feedback in the Self-Assembly and Function of Air-Liquid Interfaces: Insight into the Bottlenecks of CO₂ Direct Air Capture. *ACS Appl. Mater. Interfaces* **2023**, 15, 19634-19645 (featured on the cover).
130. Einkauf, J. D.; Williams, N. J.; Seipp, C. A.; Custelcean, R. Near Quantitative Removal of Selenate and Sulfate Anions from Wastewaters by Cocrystallization with Chelating Hydrogen-Bonding Guanidinium Ligands. *JACS Au* **2023**, 3 879-888 (featured on the cover).
129. Kasturi, A.; Jang, G. G.; Stamberg, D.; Custelcean, R.; Yiacoumi, S.; Tsouris, C. Determination of the Regeneration Energy of Direct Air Capture Solvents/Sorbents Using Calorimetric Methods, *Separation and Purification Technology* **2023**, 310, 123154.
128. Jang, G. G.; Kasturi, A.; Stamberg, D.; Custelcean, R.; Keum, J. K. Yiacoumi, S.; Tsouris, C. Ultra-fast Microwave Regeneration of CO₂ Solid Sorbents for Energy-Efficient Direct Air Capture, *Separation and Purification Technology* **2023**, 309, 123053.
127. Custelcean, R. Reducing Atmospheric Carbon Dioxide through Direct Air Capture, *ORNL Reviews* **2022**, 55, 48-51.
126. Ozkan, M.; Custelcean, R. The Status and Prospects of Materials for Carbon Capture Technologies, *MRS Bulletin* **2022**, 47, 1-5.
125. Einkauf, J. D.; Bryantsev, V. S.; Custelcean, R. Anti-Electrostatic Hydrogen-Bonded Tellurate Dimers Captured and Stabilized by Crystallization of a Bis-iminoguanidinium Salt, *Polyhedron* **2022**, 223, 115990.
124. Custelcean, R. Direct Air Capture of CO₂ Using Solvents, *Annu. Rev. Chem. Biomol. Eng.* **2022**, 13, 217-234.
123. Stamberg, D.; Thiele, N. A.; Custelcean, R. Synergistic Direct Air Capture of CO₂ with Aqueous Guanidine/Amino Acid Solvents, *MRS Advances* **2022**, 7, 399-403.
122. Einkauf, J. D.; Bryantsev, V. S.; Moyer, B. A.; Custelcean, R. A Photoresponsive Receptor with a 10⁵ Magnitude of Reversible Anion-Binding Switching, *Chem. Eur. J.* **2022**, 28, e202200719 (featured on the cover).
121. Custelcean, R. Direct Air Capture with Bis-iminoguanidines: From Discovery to Commercialization, *Chem* **2021**, 7, 2848-2852.
120. Custelcean, R. Direct Air Capture of CO₂ via Crystal Engineering, *Chem. Sci.* **2021**, 12, 12518-12528.
119. Kasturi, A.; Gabbito, J.; Custelcean, R.; Tsouris, C. A Process Intensification Approach for CO₂ Absorption Using Amino Acid Solutions and a Guanidine Compound, *Energies* **2021**, 14, 5821.
118. Kasturi, A.; Gabbito, J.; Tsouris, C.; Custelcean, R. Carbon Dioxide Capture with Aqueous Amino Acids: Mechanistic Study of Amino Acid Regeneration by Guanidine Crystallization and Process Intensification, *Separation and Purification Technology* **2021**, 271, 118839.
117. Custelcean, R.; Garrabrant, K. A.; Agullo, P.; Williams, N. J. Direct Air Capture of CO₂ with Aqueous Peptides and Crystalline Guanidines, *Cell Reports Physical Science* **2021**, 2, 100385 (featured on the cover). Highlighted in *Chemical & Engineering News*.
116. Custelcean, R. Reducing Atmospheric Carbon Dioxide Through Direct Air Capture, *Scientia*, February **2021**, Issue 138: Exciting Innovations in Physical Science and Technology, 20-23. <https://doi.org/10.33548/SCIENTIA613>.
115. Custelcean, R.; Williams, N. J.; Wang, X.; Garrabrant, K. A.; Martin, H. J.; Kidder, M. K.; Ivanov, A. S.; Bryantsev, V. S. Dialing in Direct Air Capture of CO₂ by Crystal

- Engineering of Bis-iminoguanidines*, *ChemSusChem*, **2020**, *13*, 6381-6390, invited paper for the Special Issue *Green Carbon Science: CO₂ Capture and Conversion*. Highlighted in *ChemViews*.
114. Liu, M.; Custelcean, R.; Seifert, S.; Kuzmenko, I.; Gadikota, G. *Hybrid Absorption-Crystallization Strategies for the Direct Air Capture of CO₂ Using Phase-Changing Guanidinium Bases: Insights from in Operando X-Ray Scattering and Infrared Spectroscopy Measurements*, *Ind. Eng. Chem. Res.* **2020**, *59*, 20953-20959.
 113. Thevenet, A.; Custelcean, R.; Moyer, B. A.; Jansone-Popova, S. *Synergistic Self-Assembly of Oxoanions and d-Block Metal Ions with Heteroditopic Receptors into Triple-Stranded Helicates*, *Chem. Eur. J.* **2020**, *26*, 14290-14294 (featured on the inside cover).
 112. Custelcean, R. *Iminoguanidines: From Anion Recognition and Separation to Carbon Capture*, *Chem. Commun.* **2020**, *56*, 10272-10280, invited Feature Article.
 111. Sanjeewa, L. D.; Xing, J.; Taddei, K. M.; Parker, D.; Custelcean, R.; dela Cruz, C.; Sefat, A. S. *Evidence of Ba-substitution Induced Spin-Canting in the Magnetic Weyl Semimetal EuCd₂As₂*, *Phys. Rev. B* **2020**, *102*, 104404.
 110. Xing, J.; Sanjeewa, L. D.; Kim, J.; Stewart, G. R.; Du, M.-H.; Reboredo, F. A.; Custelcean, R.; Sefat, A. S. *Crystal Synthesis and Frustrated Magnetism in Triangular Lattice CsRESe₂ (RE = La-Lu): Quantum Spin Liquid Candidates CsCeSe₂ and CsYbSe₂*, *ACS Materials Lett.* **2020**, *2*, 71-75.
 109. Xing, J.; Sanjeewa, L. D.; Kim, J.; Meier, W. R.; May, A. F.; Zheng, Q.; Custelcean, R.; Stewart, G. R.; Sefat, A. S. *Synthesis, magnetization, and heat capacity of triangular lattice materials NaErSe₂ and KErSe₂*, *Phys. Rev. Mater.* **2019**, *3*, 114413.
 108. Custelcean, R.; Williams, N. J.; Garrabrant, K. A.; Agullo. P. Brethomé F. M.; Martin, H. J.; Kidder, M. K. *Direct Air Capture of CO₂ with Aqueous Amino Acids and Solid Bis-iminoguanidines (BIGs)*, *Ind. Eng. Chem. Res.* **2019**, *58*, 23338-23346.
 107. Kasturi, A.; Ladshaw, A.; Yiacomou, S.; Gabitto, J.; Garrabrant, K.; Custelcean, R.; Tsouris, C. *CO₂ Absorption from Simulated Flue Gas in a Bubble Column*, *Sep. Sci. Tech.* **2019**, *54*, 2034-2046.
 106. Gabitto, J.; Custelcean, R.; Tsouris, C. *Simulation of Carbon Dioxide Absorption by Amino Acids in Two-Phase Batch and Bubble Column Reactors*, *Sep. Sci. Tech.* **2019**, *54*, 2013-2025.
 105. Garrabrant, K. A.; Williams, N. J.; Holguin, E.; Brethome, F. M.; Tsouris, C.; Custelcean, R. *Energy-Efficient CO₂ Capture from Flue Gas by Absorption with Amino Acids and Crystallization with a Bis-Iminoguanidine*, *Ind. Eng. Chem. Res.* **2019**, *58*, 10510-10515 (featured on the inside cover).
 104. Williams, N. J.; Roy, S.; Reynolds, C. O.; Custelcean, R. Bryantsev, V. S.; Moyer, B. A. *Enhancing Selectivity of Cation Exchange with Anion Receptors*, *Chem. Commun.* **2019**, *55*, 3590 (featured on the inside back cover).
 103. Williams, N. J.; Custelcean, R. *CO₂ Capture Going BIG*, *Carbon Capture Journal* **2019**, *68*, Mar/Apr, 4-6.
 102. Williams, N. J.; Seipp, C. A.; Brethome, F. M.; Ma, Y.-Z.; Ivanov, A. S.; Bryantsev, V. S.; Kidder, M. K.; Martin, H. J.; Holguin, E.; Garrabrant, K. A.; Custelcean, R. *CO₂ Capture via Crystalline Hydrogen-Bonded Bicarbonate Dimers*, *Chem* **2019**, *5*, 719-730. (highlighted in Science).
 101. Huang, Z.; Jia, C.; Wu, B. Jansone-Popova, S.; Seipp, C. A.; Custelcean, R. *Selective Binding of (Thio)sulfate and Phosphate in water by Quaternary Ammonium Functionalized*

- Oligo-Ureas*”, *Chem. Commun.* **2019**, *55*, 1714-1717 (featured on the inside back cover).
100. Gianopoulos, C. G.; Chua, Z.; Zhurov, V. V.; Seipp, C. A.; Wang, X.; Custelcean, R.; Pinkerton, A. A. “Direct Air Capture of CO₂ – Topological Analysis of the Experimental Electron Density (QTAIM) of the Highly Insoluble Carbonate Salt of 2,6-Pyridine-bis(iminoguanidine), (PyBIGH₂)(CO₃)(H₂O)₄”, *IUCrJ* **2019**, *6*, 56-65.
99. Stack, A. G.; Stubbs, J. E.; Srinivasan, S. G.; Roy, S.; Bryantsev, V. S.; Eng, P. J.; Custelcean, R.; Gordon, A. D.; Hexel, C. R. “Mineral-Water Interface Structure of Xenotime (YPO₄) {100}”, *J. Phys. Chem. C* **2018**, *122*, 20232.
98. Williams, N. J.; Seipp, C. A.; Garrabrant, K. A.; Custelcean, R.; Holguin, E.; Keum, J. K.; Ellis, R. J.; Moyer, B. A. “Surprisingly Selective Sulfate Extraction by a Simple Monofunctional Di(imino)guanidinium Micelle-Forming Anion Receptor”, *Chem. Commun.* **2018**, *54*, 10048.
97. Brethome, F. M.; Williams, N. J.; Seipp, C. A.; Kidder, M. K.; Custelcean, R. “Direct Air Capture of CO₂ via Aqueous-Phase Absorption and Crystalline-Phase Release Using Concentrated Solar Power”, *Nature Energy* **2018**, *3*, 553-559.
96. Jia, C.; Zuo, W.; Yang, D.; Chen, Y.; Cao, L.; Custelcean, R.; Hostas, J.; Hobza, P.; Glaser, R.; Wang, Y.-Y.; Yang, X.-J.; Wu, B. “Selective Binding of Choline by a Phosphate-Coordination-Based Triple Helicate Featuring an Aromatic Box”, *Nature Commun.* **2017**, *8*:938, DOI:10.1038/s41467-017-00915-8.
95. Jansone-Popova, S.; Ivanov, A. S.; Bryantsev, V. S.; Sloop, Jr., F. V.; Custelcean, R.; Popovs, I.; Dekarske, M. M.; Moyer, B. A. “Bis-lactam-1,10-phenanthroline (BLPhen), a New Type of Preorganized Mixed N,O-Donor Ligand That Separates Am(III) over Eu(III) with Exceptionally High Efficiency”, *Inorg. Chem.* **2017**, *56*, 5911.
94. Seipp, C. A.; Williams, N. J.; Kidder, M. K.; Custelcean, R. “CO₂ Capture from Ambient Air by Crystallization with a Guanidine Sorbent”, *Angew. Chem. Int. Ed.* **2017**, *56*, 1042-1045. (highlighted in Forbes, USA Today)
93. Seipp, C. A.; Williams, N. J.; Custelcean, R. “Sulfate Separation by Selective Crystallization with a Bis-Iminoguanidinium Ligand”, *Journal of Visualized Experiments* **2016**, *115*, e54411.
92. Sefat, A. S.; Li, L.; Cao, H. B.; McGuire, M. A.; Sales, B.; Custelcean, R.; Parker, D. S. “Anomalous Magneto-Elastic and Charge Doping Effects in Thallium-Doped BaFe₂As₂” *Scientific Reports* **2016**, *6*:21660.
91. Williams, N. J.; Bryantsev, V.; Custelcean, R.; Seipp, C. A.; Moyer, B. A. “ α , α' , α'' , α''' ” Meso-Tetrahexyltetramethyl-Calix[4]Pyrrole: An Easy-to-Prepare, Isomerically Pure Anion Extractant with Enhanced Solubility in Organic Solvents”, *Supramol. Chem.* **2016**, *28*, 176.
90. Custelcean, R.; Williams, N. J.; Seipp, C. A.; Ivanov, A. S.; Bryantsev, V. S. “Aqueous Sulfate Separation by Sequestration of [(SO₄)₂(H₂O)₄]⁴⁻ Clusters within Highly Insoluble Imine-Linked Bis-Guanidinium Crystals”, *Chem. Eur. J.* **2016**, *22*, 1997 (featured on the back cover).
89. Seipp, C. A.; Williams, N. J.; Bryantsev, V. S.; Custelcean, R.; Moyer, B. A. “A Conformationally Persistent Pseudo-Bicyclic Guanidinium for Anion Coordination, as Stabilized by Dual Intramolecular Hydrogen Bonds”, *RSC Advances* **2015**, *5*, 107266.
88. Custelcean, R.; Williams, N. J.; Seipp, C. A. “Aqueous Sulfate Separation by Crystallization of Sulfate-Water Clusters”, *Angew. Chem. Int. Ed.* **2015**, *54*, 10525 (featured on the back cover).
87. Wang, J. C.; Aswartham, S.; Ye, F.; Terzic, J.; Zheng, H.; Haskel, D.; Chikara, S.; Choi, Y.;

- Schlottmann, P.; Custelcean, R.; Yuan, S. J.; Cao, G. "Decoupling of the Antiferromagnetic and Insulating States in Tb-doped Sr_2IrO_4 ", *Phys. Rev. B*, **2015**, 92, 214411.
86. Zhuravleva, M.; Lindsey, A.; Chakoumakos, B. C.; Custelcean, R.; Meilleur, F.; Hughes, R. W.; Kriven, W. M.; Melcher, C. L. "Crystal Structure and Thermal Expansion of a $CsCe_2Cl_2$ Scintillator", *J. Solid State Chem.* **2015**, 227, 142.
85. Custelcean, R.; Sloop Jr., F. V.; Rajbanshi, A.; Wan, S.; Moyer, B. A. "Sodium Sulfate Separation from Aqueous Alkaline Solutions via Crystalline Urea-Functionalized Capsules: Thermodynamics and Kinetics of Crystallization", *Cryst. Growth Des.* **2015**, 15, 517.
84. Surowiec, M.; Custelcean, R.; Surowiec, K. Bartsch, R. A. "Alkali Metal Cation Complexation by 1,3-Alternate, Mono-ionisable Calix[4]arene-benzocrown-6 Compounds" *Supramol. Chem.* **2015**, 27, 59.
83. Fu, J.; Wu, J.; Custelcean, R.; Jiang, D.-E. "Nitrogen-Doped Porous Aromatic Frameworks for Enhanced CO_2 Adsorption", *Journal of Colloid and Interface Science* **2015**, 438, 191.
82. Jia, C.; Hay, B. P.; Custelcean, R. "De Novo Structure-Based Design of Ion-Pair Triple-Stranded Helicates", *Inorg. Chem.* **2014**, 53, 3893.
81. Custelcean, R. "Anion encapsulation and dynamics in self-assembled coordination cages", *Chem. Soc. Rev.* **2014**, 43, 1813.
80. Liao, C.; Han, K. S.; Baggetto, L.; Hillesheim, D. A.; Custelcean, R.; Lee, E.-S.; Guo, B.; Bi, Z.; Jiang, D.; Veith, G. M.; Hagaman, E. W.; Brown, G. M.; Bridges, C.; Paranthaman, M. P.; Manthiram, A.; Dai, S.; Sun, X.-G. "Synthesis and Characterization of Lithium Bis(fluoromalonato)borate for Lithium-Ion Battery Applications", *Adv. Energy Mater.* **2014**, 4.
79. Liao, C.; Guo, B.; Jiang, D.; Custelcean, R.; Mahurin, S. M.; Sun, X.-G., Dai, S. "Highly Soluble Alkoxide Magnesium Salts for Rechargeable Magnesium Batteries", *J. Mater. Chem. A.*, **2014**, 2, 581.
78. Hong, T.; Schmidt, K. P.; Coester, K.; Awwadi, F. F.; Turnbull, M. M.; Qiu, Y.; Rodriguez-Rivera, J. A.; Zhu, M.; Ke, X.; Aoyama, C. P.; Takano, Y.; Cao, H.; Tian, W.; Ma, J.; Custelcean, R.; Zhou, H. D.; Matsuda, M. "Magnetic Ordering Induced by Coupling in the Spin-1/2 Heisenberg Two-Leg Ladder Antiferromagnet $C_9H_{18}N_2CuBr_4$ " *Phys. Rev. B* **2014**, 89, 174432.
77. Rajbanshi, A.; Wan, S.; Custelcean, R. "Dihydrogen Phosphate Clusters: Trapping $H_2PO_4^-$ Tetramers and Hexamers in Urea-Functionalized Molecular Crystals", *Cryst. Growth Des.* **2013**, 13, 2233.
76. Custelcean, R. "Urea-Functionalized Crystalline Capsules for Recognition and Separation of Tetrahedral Oxoanions", *Chem. Commun.* **2013**, 49, 2173 (featured on the cover).
75. Moyer, B. A.; Custelcean, R.; Hay, B. P.; Sessler, J. L.; Bowman-James, K.; Day, V. W.; Kang, S.-O. "A Case for Molecular Recognition in Nuclear Separations: Sulfate Separation from Nuclear Wastes", *Inorg. Chem.* **2013**, 52, 3473.
74. Karki, A. B.; Garlea, O. V.; Custelcean, R.; Stadler, S.; Plummer, E. W.; Jin, R. "Interplay Between Superconductivity and Magnetism in $Fe_{1-x}Pd_xTe$ ", *Proc. Nat. Acad. Sci.* **2013**, 110, 9283.
73. Cao, H.; Chakoumakos, B. C.; Chen, X.; Yan, J.; McGuire, M. A.; Yang, H.; Custelcean, R.; Zhou, H.; Singh, D. J.; Mandrus, D. "Origin of the phase transition in $IrTe_2$: Structural Modulation and Local Bonding Instability", *Phys. Rev. B.* **2013**, 88, 115122.
72. Boatner, L. A.; Neal, J. S.; Ramey, J. O.; Chakoumakos, B. C.; Custelcean, R. "The Observation of Scintillation in a Hydrated Inorganic Compound: $CeCl_3 \cdot 6H_2O$ ", *Appl. Phys.*

Lett. **2013**, *103*, 141909.

71. Boatner, L. A.; Neal, J. S.; Ramey, J. O.; Chakoumakos, B. C.; Custelcean, R.; van Loef, E. V. D.; Markosyan, G.; Shah, K. S. "New Cerium-Based Metal-Organic Scintillators for Radiation Detection", *Nuclear Instruments and Methods in Physics Research A*, **2013**, *703*, 138.
70. Babarao, R.; Custelcean, R.; Hay, B. P.; Jiang, D. "Computer-Aided Design of Interpenetrated Tetrahydrofuran-Functionalized 3D Covalent Organic Frameworks for CO₂ Capture", *Cryst. Growth. Des.* **2012**, *12*, 5349.
69. Custelcean, R.; Bonnesen, P. V.; Roach, B. D.; Duncan, N. C. "Ion-Pair Triple Helicates and Mesocates Self-Assembled from Ditopic 2,2'-Bipyridine-bis(urea) Ligands and Ni(II) or Fe(II) Sulfate Salts", *Chem. Commun.* **2012**, *48*, 7438 (featured on the back cover).
68. Custelcean, R.; Bonnesen, P. V.; Duncan, N. C.; Zhang, X.; Watson, L. A.; Van Berkel, G.; Parson, W. B.; Hay, B. P. "Urea-Functionalized M₄L₆ Cage Receptors: Anion-Templated Self-Assembly and Selective Guest Exchange in Aqueous Solutions", *J. Am. Chem. Soc.* **2012**, *134*, 8525.
67. Rajbanshi, A.; Moyer, B. A.; Custelcean, R. "Sulfate Separation from Hanford Waste Simulants by Selective Crystallization of Urea-Functionalized Capsules", *Sep. Sci. Technology*, **2012**, *47*, 2145.
66. Custelcean, R. "Dynamic Chemistry of Anion Recognition", *Top. Curr. Chem.* **2012**, *322*, 193.
65. Rajbanshi, A.; Custelcean, R. "Structure and Selectivity Trends in Crystalline Urea-Functionalized Anion-Binding Capsules", *Supramol. Chem.* **2012**, *24*, 65.
64. Marc, P.; Custelcean, R.; Groenewold, G. S.; Klaehn, J. R.; Peterman, D. R.; Delmau, L. H. "Degradation of CYANEX 301 in Contact with Nitric Acid Media", *Ind. Eng. Chem. Res.* **2012**, *51*, 13238.
63. Groenewold, G. S.; Peterman, D. R.; Klaehn, J. R.; Delmau, L. H.; Marc, P.; Custelcean, R. "Oxidative Degradation of bis(2,4,4-trimethylpentyl)dithiophosphinic acid in nitric acid studied by electrospray ionization mass spectrometry", *Rapid Commun. Mass Spectrom.* **2012**, *26*, 2195.
62. Kang, S. O.; Vukovic, S.; Custelcean, R.; Hay, B. P. "Cyclic Imide Dioximes: Formation and Hydrolytic Stability", *Ind. Eng. Chem. Res.* **2012**, *51*, 6619.
61. Vukovic, S.; Watson, L. A.; Kang, S. O.; Custelcean, R.; Hay, B. P. "How Amidoximate Binds the Uranyl Cation", *Inorg. Chem.* **2012**, *51*, 3855.
60. Duncan, N. C.; Hay, B. P.; Hagaman, E. W.; Custelcean, R. "Thermodynamic, Kinetic, and Structural Factors in the Synthesis of Imine-Linked Dynamic Covalent Frameworks", *Tetrahedron* **2012**, *68*, 53.
59. Vaughn, S. A.; Chakoumakos, B. C.; Custelcean, R.; Ramey, J. O.; Smith, M. D.; Boatner, L. A.; zur Loye, H.-C. "New Family of Cerium Halide Based Materials: CeX₃·ROH Compounds Containing Planes, Chains, and Tetradecanuclear Rings", *Inorg. Chem.* **2012**, *51*, 10503.
58. Chakoumakos, B. C.; Custelcean, R.; Ramey, J. O.; Boatner, L. A. "New Crystal Structural Families of Lanthanide Chloride-Alcohol/Water Complexes", *Inorg. Chim. Acta* **2012**, *384*, 23.
57. Garlea, V. O.; Jin, R.; Garlea, E.; Ehlers, G.; Mamontov, E.; Myers, D. B.; Xie, F.; Custelcean, R., "Structural and Magnetic Properties of the Cobaltate Series (Ba,Sr)_{4-x}La_{2x}Co₄O₁₅", *Phys. Rev. B* **2012**, *86*, 094434.
56. Yankova, T.; Huvonen, D.; Muhlbauer, S.; Schmidiger, D.; Wulf, E.; Zhao, S.; Zheludev, A.;

- Hong, T.; Garlea, V. O.; Custelcean, R.; Ehlers, G. “Crystals for Neutron Scattering Studies of Quantum Magnetism”, *Philosophical Magazine*, **2012**, 92, 2629.
55. Ye, F.; Chi, S.; Cao, H.; Chakoumakos, B. C.; Fernandez-Baca, J. A.; Custelcean, R.; Qi, T. F.; Korneta, O. B.; Cao, G. “Direct Evidence of a Zigzag Spin-Chain Structure in the Honeycomb Lattice: A neutron and X-Ray Diffraction Investigation of a Single-Crystal Na_2IrO_3 ”, *Phys. Rev. B* **2012**, 85, 180403.
54. Cao, H.; Cantoni, C.; May, A. F.; McGuire, M. A.; Chakoumakos, B. C.; Pennycook, S. J.; Custelcean, R.; Sefat, A. S.; Sales, B. C. “Evolution of the Nuclear and Magnetic Structures of $\text{TlFe}_{1.6}\text{Se}_2$ with Temperature”, *Phys. Rev. B* **2012**, 85, 054515.
53. May, A. F.; McGuire, M. A.; Ma, J.; Delaire, O.; Huq, A.; Custelcean, R. “Properties of Single Crystalline AZn_2Sb_2 ($A = \text{Ca}, \text{Eu}, \text{Yb}$)”, *J. Appl. Phys.* **2012**, 111, 033708.
52. May, A. F.; McGuire, M. A.; Singh, D. J.; Custelcean, R.; Jellison Jr., G. E. “Structure and Properties of Single Crystalline CaMg_2Bi_2 , EuMg_2Bi_2 , and YbMg_2Bi_2 ,” *Inorg. Chem.* **2011**, 50, 11127.
51. Rajbanshi, A.; Moyer, B. A.; Custelcean, R. “Sulfate Separation from Aqueous Alkaline Solutions by Selective Crystallization of Alkali Metal Coordination Capsules”, *Cryst. Growth Des.* **2011**, 11, 2702.
50. Borman, C. J.; Custelcean, R.; Hay, B. P.; Bill, N. L.; Sessler, J. L.; Moyer, B. A. “Supramolecular Organization of Calix[4]Pyrolle with a Methyl-trialkylammonium Anion Exchanger Leads to Remarkable Reversal of Selectivity for Sulfate Extraction vs. Nitrate”, *Chem. Commun.* **2011**, 47, 7611.
49. Custelcean, R. “Anions in Crystal Engineering”, *Chem. Soc. Rev.* **2010**, 39, 3675.
48. Custelcean, R.; Bock, A.; Moyer, B. A. “Selectivity Principles in Anion Separation by Crystallization of Hydrogen-Bonding Capsules”, *J. Am. Chem. Soc.* **2010**, 132, 7177.
47. Neal, J. S.; Boatner, L. A.; Bell, Z. W.; McConchie, S. M.; Wisniewski, D.; Ramey, J. O.; Kolupus, J. A.; Chakoumakos, B. C.; Wisniewska, M.; Custelcean, R.; “A New Scintillator for fast Neutron Detection: Single-Crystal $\text{CeCl}_3(\text{CH}_3\text{OH})_4$ ”, *IEEE Transactions on Nuclear Science* **2010**, 57, 1692.
46. Hong, T.; Custelcean, R.; Sales, B. C.; Roessli, D.; Singh, D. K.; Zheludev, A. “Synthesis and Structural Characterization of $2\text{Dioxane}\cdot 2\text{H}_2\text{O}\cdot \text{CuCl}_2$: Metal-Organic Compound with Heisenberg antiferromagnetic $S=1/2$ Chains”, *Phys. Rev. B* **2009**, 80, 132404.
45. Boatner, L. A.; Wisniewski, D.; Neal, J. S.; Bell, Z. W.; Ramey, J. O.; Kolupus, J. A.; Chakoumakos, B. C.; Wisniewska, M.; Custelcean, R.; Wisniewska, M.; Pena, K. E., “Rare-Earth Tri-Halide Methanol-Adduct Single-Crystal Scintillators for Gamma Ray and Neutron Detection”, *SPIE Optics and Photonics Proceedings* **2009**, Vol. 7449.
44. Surowiec, M.; Custelcean, R.; Surowiec, K.; Bartsch, R. A., “Mono-Ionizable Calix[4]arene-benzocrown-6 Ligands in 1,3-Alternate Conformation: Synthesis, Structure and Silver(I) Extraction”, *Tetrahedron* **2009**, 65, 7777.
43. Loustau-Chartez, F.; Robeson, R. M.; Custelcean, R.; Sachleben, R. A.; Bonnesen, P. V., “2,2,3,3,11,11,12,12-Octamethyl-1,4,7,10,13-Pentaoxacyclohexadecane: Improved Synthesis and Crystal Structure with NaSCN ”, *Tetrahedron Letters* **2009**, 50, 2936.
42. Custelcean, R., “Ion Separation by Selective Crystallization of Organic Frameworks”, *Curr. Opin. Solid State Mater. Sci.* **2009**, 13, 68 (invited review), **top 20 most cited papers 2007–2011**.
41. Hay, B. P.; Custelcean, R., “Anion- π Interactions: Commonplace or Extraordinary?”, *Cryst. Growth Des.* **2009**, 9, 2539, **featured on the cover**.

40. Custelcean, R.; Bosano, J.; Bonnesen, P. V.; Kertesz, V.; Hay, B. P., “Computer-Aided Design of a Sulfate Encapsulating Receptor”, *Angew. Chem. Int. Ed.* **2009**, *48*, 4025. **highlighted in Chemistry World, April 27, 2009.**
39. Custelcean, R.; Remy, P., “Selective Crystallization of Urea-Functionalized Capsules with Tunable Anion-Binding Cavities”, *Cryst. Growth Des.* **2009**, *9*, 1985-1989.
38. Boatner, L. A.; Wisniewski, D.; Neal, J. S.; Ramey, J. O.; Kolopus, J. A.; Chakoumakos, B. C.; Wisniewska, M.; Custelcean, R. “Single-Crystal $CeCl_3(CH_3OH)_4$: A new metal-organic cerium chloride methanol adduct for scintillator applications”, *Applied Physics Letters* **2008**, *93*, 244104.
37. Chakoumakos, B. C.; Custelcean, R.; Ramey, J. O.; Kolopus, J. A.; Jin, R.; Neal, J. S.; Wisniewski, D. J.; Boatner, L. A. “Cerium chloride – methanol adduct crystals, $CeCl_3(CH_3OH)_4$: preparation, crystallography, and scintillation properties”, *Cryst. Growth Des.* **2008**, *8*, 2070.
36. Custelcean, R.; Jiang, D.; Hay, B. P.; Luo, W.; Gu, B. “Hydrogen-Bonded Helices for Anion Binding and Separation”, *Cryst. Growth Des.* **2008**, *8*, 1909, **featured on the cover.**
35. Custelcean, R.; Remy, P.; Bonnesen, P. V.; Jiang, D.-E.; Moyer, B. A. “Sulfate Recognition by Persistent Crystalline Capsules with Rigidified Hydrogen Bonding Cavities”, *Angew. Chem. Int. Ed.* **2008**, *47*, 1866.
34. Custelcean, R. “Crystal Engineering with Urea and Thiourea Hydrogen-Bonding Groups”, *Chem. Commun.* **2008**, 295 (invited Feature Article), **top 10 most accessed papers, 01/2008.**
33. Custelcean, R.; Engle, N. L.; Bonnesen, P. V. “Crystalline Hydrogen-Bonded Nanocolumns of Cyclic Thiourea Octamers”, *CrystEngComm* **2007**, *9*, 452 (invited paper for the special issue: “Crystal Engineering in the Design of New Materials”), **top 10 most accessed papers, 06/2007.**
32. Custelcean, R.; Moyer, B. A. “Anion Separation with Metal-Organic Frameworks” invited review, *Eur. J. Inorg. Chem.* **2007**, *10*, 1321 (**featured on the cover, most accessed paper in 03/07, 2nd most cited in 2009**).
31. Custelcean, R.; Sellin, V.; Moyer, B. A. “Sulfate Separation by Selective Crystallization of a Urea-Functionalized Metal-Organic Framework” *Chem. Commun.* **2007**, 1541.
30. Chakoumakos, B. C.; Custelcean, R.; Kamiyama, T.; Oikawa, K.; Sales, B. C.; Lumsden, M. D. “Structural Modulation in $K_2V_3O_8$ ” *J. Solid State Chem.* **2007**, *180*, 812.
29. Custelcean, R.; Haverlock, T. J.; Moyer, B. A. “Anion Separation by Selective Crystallization of Metal-Organic Frameworks” *Inorg. Chem.* **2006**, *45*, 6446.
28. Custelcean, R.; Moyer, B. A.; Bryantsev, V. S.; Hay, B. P. “Anion Coordination in Metal-Organic Frameworks Functionalized with Urea Hydrogen-Bonding Groups” *Cryst. Growth Des.* **2006**, *6*, 555 (**top 10 most cited papers in 2006**).
27. Custelcean, R.; Moyer, B. A.; Hay, B. P. “A Coordinatively Saturated Sulfate Encapsulated in a Metal-Organic Framework Functionalized with Urea Hydrogen-Bonding Groups” *Chem. Commun.* **2005**, 5971 (**featured on the cover**).
26. Custelcean, R.; Gorbunova, M. G. “A Metal-Organic Framework Functionalized with Free Carboxylic Acid Sites and its Selective Binding of a $Cl(H_2O)_4^-$ Cluster” *J. Am. Chem. Soc.* **2005**, *127*, 16362.
25. Vlassa, M.; Custelcean, R.; Jackson, J. E. “Construction of Self-Assembled Nanostructures by Means of Dihydrogen Bonding” in *Nanostructures: Novel Architectures*, Ed. Diudea, M., Nova Publishers, **2005**.
24. Custelcean, R.; Gorbunova, M. G. “Protonation-Assisted Spontaneous Resolution: Formation

- of a Homochiral 2D Interpenetrated Hydrogen-Bonded Network from 4,4'-Bimicoticinic Acid under Highly Acidic Conditions" *CrystEngComm*. **2005**, *7*, 297.
23. Custelcean, R.; Ward, M. D. "Chiral Discrimination in Low-Density Hydrogen-Bonded Frameworks" *Cryst. Growth Des.* **2005**, *5*, 2277 (top 10 most accessed papers, October-December/2007).
 22. Custelcean, R.; Delmau, L. H.; Moyer, B. A.; Sessler, J. L.; Cho, W.-S.; Gross, D.; Bates, G. W.; Brooks, S. J.; Light, M. E.; Gale, P. A. "Calix[4]pyrrole: An Old yet New Ion-Pair Receptor" *Angew. Chem. Int. Ed.* **2005**, *44*, 2537 (featured on the cover).
 21. Custelcean, R.; Gorbunova M. G.; Bonnesen, P. V. "Steric Control over Hydrogen Bonding in Crystalline Organic Solids: A Structural Study of N,N'-Dialkylthioureas" *Chem. Eur. J.* **2005**, *11*, 1459.
 20. Moyer, B. A.; Bonnesen, P. V.; Custelcean, R.; Delmau, L. H.; Hay, B. P. "Strategies for Using Host-Guest Chemistry in the Extractive Separation of Ionic Guests" *Kem. Ind.* **2005**, *54*, 65.
 19. Marincean, S.; Custelcean, R.; Stein, R. S.; Jackson, J. E. "Structural Reinvestigation of Ammonium Hypophosphite: Was Dihydrogen Bonding Observed Long Ago?" *Inorg. Chem.* **2005**, *44*, 45.
 18. Custelcean, R.; Dreger, Z. A. "Dihydrogen Bonding under High Pressure: A Raman Study of BH₃NH₃ Molecular Crystal" *J. Phys. Chem. B* **2003**, *107*, 9231.
 17. Bader, M. M.; Custelcean, R.; Ward, M. D. "Tricyanovinyl-Substituted Oligothiophenes" *Chem. Mater.* **2003**, *15*, 616.
 16. Custelcean, R.; Ward, M. D. "Hydrogen-Bonded Helices in Crystals with Prescribed Organization" *Angew. Chem. Int. Ed.* **2002**, *41*, 1724.
 15. Custelcean, R.; Vlassa, M.; Jackson, J. E. "Supramolecular Synthesis through Dihydrogen Bonds: Self-Assembly of Controlled Architectures from NaBH₄·Poly(2-hydroxyethyl)cyclen Building Blocks" *Chem. Eur. J.* **2002**, *8*, 302.
 14. Custelcean, R.; Jackson, J. E. "A Mechanistic Study of a Topochemical Dihydrogen to Covalent Bonding Transformation" *Thermochimica Acta* **2002**, *388*, 143.
 13. Custelcean, R.; Jackson, J. E. "Dihydrogen Bonding: Structures, Energetics, and Dynamics" *Chem. Rev.* **2001**, *101*, 1963.
 12. Custelcean, R.; Vlassa, M.; Jackson, J. E. "Toward Crystalline Covalent Solids: Crystal-to-Crystal Dihydrogen to Covalent Bonding Transformation in NaBH₄·THEC" *Angew. Chem. Int. Ed.* **2000**, *39*, 3299.
 11. Custelcean, R.; Jackson, J. E. "Topochemical Dihydrogen to Covalent Bonding Transformation in LiBH₄·TEA: A Mechanistic Study" *J. Am. Chem. Soc.* **2000**, *122*, 5251.
 10. Custelcean, R.; Afloroaiei, C.; Vlassa, M.; Polverejan, M. "Formation of Extended Tapes of Cyclic Water Hexamers in an Organic Molecular Crystal Host" *Angew. Chem. Int. Ed.* **2000**, *39*, 3094.
 9. Custelcean, R.; Craciun, L. "3-Ethyl-6-methyl-isocytosines: Synthesis and Solid State Structural Analysis" *Tetrahedron*, **2000**, *56*, 5067.
 8. Custelcean, R. "Ab Initio Comparative Study of BH₄CN and BH₅" *J. Mol. Struct. Theochem* **2000**, *505*, 95.
 7. Craciun, L.; Custelcean, R. "Syntheses and Crystal Structures of 9-Acetyl- and 9-Cyano-1,2-dicarbododecaborane: Supramolecular Association in Carboranyl C-H Hydrogen-Bonded α -Networks" *Inorg. Chem.* **1999**, *38*, 4916.
 6. Craciun, L.; Custelcean, R.; Mager, S. "Molecular Structure of an Isocytosine Analog:

- Combined X-ray Structural and Computational Study of 2-Diethylamino-6-methyl-5-*n*-propyl-4(3*H*)-pyrimidinone" *Struct. Chem.* **1999**, *10*, 303 (featured on the cover).
5. Custelcean, R.; Jackson, J. E. "Tuning Dihydrogen Bonds: Enhanced Solid-State Reactivity in a Dihydrogen-Bonded System with Exceptionally Short H...H Distances" *Angew. Chem. Int. Ed.* **1999**, *38*, 1661.
 4. Custelcean, R.; Jackson, J. E. "Topochemical Control of Covalent Bond Formation by Dihydrogen Bonding" *J. Am. Chem. Soc.* **1998**, *120*, 12935.
 3. Custelcean, R.; Vlassa, M.; Silberg, I. A. "Reaction of π -Deficient Aromatic Heterocycles with Ammonium Polyhalides. III. Halogenation of Phenothiazin-5-oxide with Benzyltriethylammonium Polyhalides" *Monatsh. Chem.* **1997**, *128*, 919.
 2. Custelcean, R.; Vlassa, M.; Silberg, I. A.; Szoke, M.; Farcas, S. I.; Culea, M. "Reaction of π -Deficient Aromatic Heterocycles with Ammonium Polyhalides. II. Halogenation of Phenothiazine with Benzyltriethylammonium (BTEA) Polyhalides" *Heterocyclic Comm.* **1997**, *3*, 317.
 1. Vlassa, M.; Silberg, I. A.; Custelcean, R.; Culea, M. "Reaction of π -Deficient Aromatic Heterocycles with Ammonium Polyhalides. I. Halogenation of Acridone and Acridine with Benzyltriethylammonium (BTEA) Polyhalides" *Synth. Comm.* **1995**, *25*, 3493.

Patents:

Williams, N. J.; Custelcean, R.; Seipp, C. A.; Moyer, B. A.; Ellis, R.; Abney, C. W. *Lipophilic Guanidinium Compounds for Removal of Oxyanions from Aqueous Solutions*, US patent number 11,001,554, granted on May 11, **2021**.

Custelcean, R.; Seipp, C. A.; Williams, N. J. "*Guanidine Compounds for Removal of Oxyanions from Aqueous Solutions and for Carbon Dioxide Capture*", US patent number 10,633,332, granted on April 28, **2020**.

Custelcean, R.; Seipp, C. A.; Williams, N. J. "*Guanidine Compounds for Carbon Dioxide Capture*", US patent number 10,583,387, granted on March 10, **2020**.

Custelcean, R.; Moyer, B. A.; Rajbanshi, A. "*Selective Oxoanion Separation Using a Tripodal Ligand*", US patent number 9,260,326, granted on February 16, **2016**.

Presentations:

- 85.
84. Custelcean, R. *Direct Air Capture of CO₂ with Aqueous Amino Acids or Peptides and Crystalline Guanidines*, invited talk, ACS Spring Meeting, Indianapolis, Mar 28, **2023**.
83. Custelcean, R. *Solving Energy and Environmental Problems via Crystal Engineering with Guanidines*, invited seminar, University of South Dakota, November 7, **2022**.
82. Custelcean, R.; Stamberg, D.; Tsouris, C.; Jang, G. G.; An, K.; Nawaz, K.; Kasturi, A.; Iglesias, B. *Integrated Process for Direct Air Capture of CO₂ and Electrochemical Conversion to Ethanol*, invited poster presentation, 2022 Carbon Management Project Review Meeting, Pittsburgh, PA, August 15-19, **2022**.

81. Custelcean, R. *Selective Separation of Se Oxyanions by Chelating Hydrogen-Bonding Ligands*, invited presentation, *NAWI Biannual Review (online)*, April 28, 2022.
80. Custelcean, R. *BIG NET: An Energy-Efficient & Sustainable Technology for Removing CO₂ out of the Atmosphere*, invited seminar, Michigan State University, June 30, **2022**.
79. Custelcean, R. *BIG NET: An Energy-Efficient & Sustainable Technology for Removing CO₂ out of the Atmosphere*, invited BASF seminar, Wyandotte MI, June 28, **2022**.
78. Custelcean, R. “*Iminoguanidines: From Anion Recognition and Separation to Carbon Capture*”, Pacificchem 2021 (virtual conference), Anion Recognition Chemistry Symposium, December 18, **2021**.
77. Custelcean, R. “*Direct Air Capture of CO₂ with Aqueous Amino Acids/Peptides and Crystalline Guanidines*”, 2021 MRS Fall Meeting (virtual), Climate Change Mitigation Technologies Symposium, December 6, **2021**.
76. Custelcean, R. “*Iminoguanidines: From Anion Recognition and Separation to Carbon Capture*”, Separation Science PI Meeting, U.S. Department of Energy, Office of Science, Basic Energy Sciences, August 10-12, **2021**, invited presentation.
75. Custelcean, R. “*Integrated process for Direct Air Capture of CO₂ and its Electrochemical Conversion to Ethanol*”, NETL-FE Direct Air Capture Virtual Kickoff Meeting, Feb 24-25, **2021**, invited presentation.
74. Custelcean, R. “*Direct Air Capture of CO₂ with Aqueous Amino Acids and Crystalline Bis-iminoguanidines (BIGs)*”, NETL-FE Direct Air Capture Virtual Kickoff Meeting, Feb 24-25, **2021**, invited presentation.
73. Custelcean, R. “*Direct Air Capture of CO₂ with Aqueous Amino Acids and Crystalline Guanidines*”, Gordon Research Conference on Chemical Separations, Jan 26-31, **2020**, Galveston, TX, poster presentation.
72. Custelcean, R. “*From Cluj to Oak Ridge: Solving Energy and Environmental Problems with Crystal Engineering*”, Chemia Napocensis – 100, October 9-12, **2019**, Cluj-Napoca, Romania, invited presentation.
71. Custelcean, R. “*Principles of Chemical Recognition and Transport in Extractive Separations: The Iminoguanidinium Group as Versatile Oxoanion Recognition Unit*”, Separation Science Research PI Meeting, September 9-11, **2019**, Gaithersburg, Maryland, invited presentation.
70. Custelcean, R. “*CO₂ Separation by Guanidines Crystallization*”, Separation Science Research PI Meeting, September 9-11, **2019**, Gaithersburg, Maryland, poster presentation.
69. Custelcean, R. “*CO₂ Separation by Guanidines Crystallization*”, Georgia Institute of Technology, August 15, **2019**, invited seminar.
68. Custelcean, R. “*CO₂ Separation by Guanidines Crystallization*”, ICCOSS XXIV, June 16-21, **2019**, New York City, NY, poster presentation.
67. Custelcean, R. “*CO₂ Separation by Guanidines Crystallization*”, Gordon Research Conference, Carbon Capture Utilization and Storage, May 5-10, **2019**, Les Diablerets, Switzerland, poster presentation.
66. Custelcean, R. “*CO₂ Separation by Guanidine Crystallization*”, ACS Spring 2019 National Meeting, I&EC Symposium in honor of Sheng Dai, March 31, **2019**, Orlando, FL, invited presentation.
65. Custelcean, R. “*Direct Air Capture of CO₂*”, Friends of ORNL, UT Resource Center, Oak Ridge, TN, Nov. 13, **2018**, invited presentation.
64. Custelcean, R. “*Anion Separation by Selective Crystallization*”, University of California at

- Santa Cruz, Oct. 8, **2018**, Chemistry Department seminar presentation.
63. Custelcean, R. "*CO₂ Capture via Crystallization with Guanidines*", Gordon Research Conference, Crystal Engineering, June 28, **2018**, Newry Maine, invited presentation.
 62. Custelcean, R. "*Aqueous Ion Separations by Selective Crystallization*", National Academy of Sciences, A Research Agenda for a New Era in Separations Science, May 8, **2018**, Irvine, CA, invited presentation.
 61. Custelcean, R. "*Confinement of Anion-Water Clusters in Guanidine Crystals*", 255th ACS National Meeting, Molecular Confinement Effects in Inorganic & Organic Containers Symposium, March 20-21, **2018**, New Orleans, invited presentation.
 60. Custelcean, R. "*Selective Crystallization of Anion-Water Clusters with Self-Assembled Guanidines*", 254th ACS National Meeting, Structural & Supramolecular Aspects of Ion Separations Symposium, August 21, **2017**, Washington DC, invited presentation.
 59. Custelcean, R. "*Selective Crystallization of Oxoanion-Water Clusters with Self-Assembled Guanidine Ligands*", 12th International Symposium on Macrocyclic and Supramolecular Chemistry, July 2-6, **2017**, Cambridge, UK, invited keynote presentation.
 58. Custelcean, R.; Seipp, C. A.; Williams, N. J.; Kidder, M. K.; Xiaoping, W. "*CO₂ Capture from Ambient Air via Crystallization with Guanidine Ligands*", Carbon Capture, Utilization & Storage, Gordon Research Conference, June 11-16, **2017**, Colby-Sawyer College, New London, NH, poster presentation.
 57. Custelcean, R. "*Selective Crystallization of Anion-Water Clusters with Self-Assembled Guanidines*", Separations and Heavy Element Chemistry, DOE Contractors' Meeting, April 23-26, **2017**, Gaithersburg, Maryland, invited oral presentation.
 56. Custelcean, R.; Seipp, C. A. Williams, N. J.; Ivanov, A. S.; Bryantsev, V. S. "*Anion Separation by Selective Crystallization of Anion-Water Clusters with Self-Assembled Guanidinium Receptors*", The 68th Southeastern Regional Meeting of the American Chemical Society (SERMACS), Molecules to Functional Supramolecular Materials Symposium, October 25, **2016**, Columbia, South Carolina, invited oral presentation.
 55. Custelcean, R.; Seipp, C. A. Williams, N. J.; Ivanov, A. S.; Bryantsev, V. S. "*Anion Separation by Selective Crystallization of Anion-Water Clusters with Self-Assembled Guanidinium Receptors*", Crystal Engineering Gordon Research Conference, June 26 – July 1, **2016**, Stowe, Vermont, poster presentation.
 54. Custelcean, R. "*Aqueous Anion Separation by Selective Crystallization of Self-Assembled Guanidinium Receptors*", Anion Receptors Symposium, PacifiChem 2015, December 19, **2015**, Honolulu, Hawaii, invited oral presentation.
 53. Custelcean, R.; Bonnesen, P. V.; Jansone-Popova, S.; Jia, C.; Hay, B. P.; Moyer, B. A. "*Self-Assembled Architectures via Ion-Pair Coordination*", *Separations and Heavy Element Chemistry*, DOE Contractors' Meeting, April 19-22, **2015**, Gaithersburg, Maryland, invited poster presentation.
 52. Custelcean, R.; Sloop Jr., F. V.; Rajbanshi, S.; Wan, S.; Moyer, B. A. "*Sodium Sulfate Separation from Aqueous Alkaline Solutions via Crystalline Urea-Functionalized Capsules: Thermodynamics and Kinetics of Crystallization*" 18th Symposium on Separation Science and Technology for Energy Applications, October 27-30, **2014**, Oak Ridge, Tennessee, oral presentation.
 51. Custelcean, R.; Bonnesen, P. V.; Jia, C.; Hay, B. P. "*Self-Assembled Architectures via Ion-Pair Coordination*" American Chemical Society Meeting, August 10-14, **2014**, San Francisco, invited presentation.

50. Custelcean, R.; Bonnesen, P. V.; Roach B. D.; Duncan, N. C., Hay, B. P. “*Ion-Pair Recognition in Self-Assembled Helicates*”, *8th International Symposium on Macrocyclic and Supramolecular Chemistry*, Arlington, Virginia, July 7-11, **2013**, poster presentation.
49. Custelcean, R.; Bonnesen, P. V.; Hay, B. P.; Moyer, B. A. “*Ion-Pair Recognition and Separation via Self-Assembly*, *Separations and Heavy Element Chemistry*, DOE Contractors’ Meeting, April 21-24, **2013**, Gaithersburg, Maryland, invited poster presentation.
48. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Eastern Illinois University, September 12, **2012**, invited seminar.
47. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Materials and Chemistry Seminar, Oak Ridge National Laboratory, August 22, **2012**, invited seminar.
46. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Zhejiang University, Hangzhou, China, May 8, **2012**, invited seminar.
45. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Northwest University, Xi’an, China, May 5, **2012**, invited seminar.
44. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Nanjing University, Nanjing, China, May 3, **2012**, invited seminar.
43. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Shanghai University, Shanghai, China, May 2, **2012**, invited seminar.
42. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Michigan State University, March 27, **2012**, invited seminar.
41. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, Western Michigan University, March 26, **2012**, invited seminar.
40. Custelcean, R.; Rajbanshi, A.; Moyer, B. A. “*Self-Assembled Capsule Receptors for Sulfate Recognition and Separation*”, *17th Symposium on Separation Science and Technology for Energy Applications*, October 23-27, **2011**, Gatlinburg, TN, oral presentation.
39. Custelcean, R. “*Self-Assembled Cage Receptors for Anion Recognition and Separation*”, *6th International Symposium on Macrocyclic and Supramolecular Chemistry*, Brighton, UK, July 3-7, **2011**, invited keynote presentation.
38. Custelcean, R. “*Engineering Crystals for Nuclear Energy and Environmental Applications*”, *American Crystallographic Association Meeting*, New Orleans, May 28-June 2, **2011**, invited presentation.
37. Custelcean, R.; Moyer, B. A.; Hay, B. P., Bonnesen, P. V.; “*Selectivity Principles in Anion Separation by Self-Assembled Cage Receptors*”, *Separations and Heavy Element Chemistry*, DOE Contractors’ Meeting, April 26-29, **2011**, Baltimore, Maryland, oral presentation.
36. Custelcean, R.; Duncan, N.; Hay, B. P. “*Self-Assembly of Dynamic Covalent Cages and Frameworks*”, *Pacificchem 2010*, Hawaii, invited presentation.
35. Custelcean, R. “*Anion Recognition and Separation with Self-Assembled Cage Receptors*”, *Pacificchem 2010*, Hawaii, invited presentation.
34. Custelcean, R.; Bonnesen, P. V.; Bosano, J.; Hay, B. P.; Duncan, N. "Self-Assembled Cage Receptors for Anion Recognition and Separation", *American Chemical Society Meeting*, March 23-24 , **2010**, San Francisco, invited presentation.
33. Custelcean, R.; Bock, A.; Bosano, J.; Remy, P.; Bonnesen, P. V.; Hay, B. P.; Moyer, B. A. "Anion Recognition and Separation with Self-Assembled Cage Receptors", *Midwest ACS Meeting, October 21-24, 2009*, Iowa City, IA, invited presentation.
32. Custelcean, R.; Bock, A.; Bonnesen, P. V.; Moyer, B. A. "Sulfate Separation by Selective

- Crystallization of Hydrogen-Bonded Capsules", *16th Symposium on Separation Science & Technology for Energy Applications*, October 18-22, **2009**, Gatlinburg, TN, oral presentation.
31. Custelcean, R.; Bosano, J.; Remi, P.; Bock, A.; Moyer, B. A.; Hay, B. P., Bonnesen, P. V.; Delmau, L. H. "Anion Recognition and Separation with Self-Assembled Cage Receptors", *DOE Contractors' Meeting*, April 21-24, **2009**, Warrenton, Virginia, poster presentation.
 30. Custelcean, R. "Manipulating Hydrogen Bonds in Crystalline Solids: From Etter's Rules to Anion Recognition", Margaret Etter award symposium, *American Crystallographic Association Meeting*, May 31-June 5, **2008**, Knoxville, keynote presentation.
 29. Custelcean, R.; Remy, P.; Sellin, V.; Bonnesen, P. V.; Moyer, B. A. "Metal-Organic Frameworks Functionalized with Urea Hydrogen-Bonding Groups for Selective Anion Separation", Symposium: *Metal-Organic Frameworks: What Are They Good For?*, *American Chemical Society Meeting*, April 6-10, **2008**, New Orleans, oral presentation.
 28. Custelcean, R.; Remy, P.; Sellin, V.; Bonnesen, P. V.; Moyer, B. A. "Anion Separation by Selective Crystallization of Metal-Organic Frameworks", *15th Symposium on Separation Science & Technology for Energy Applications*, October 21-25, **2007**, Gatlinburg, TN, poster presentation.
 27. Custelcean, R.; Sellin, V., Remy, P.; Bonnesen, P. V.; Hay, B. P.; Moyer, B. A. "Anion Coordination and Separation with Metal-Organic and Hydrogen-Bonded Frameworks", *Anion Coordination Symposium, American Chemical Society Meeting*, August 19-23, **2007**, Boston, invited presentation.
 26. Custelcean, R.; Sellin, V., Moyer, B. A. "Coordination and Hydrogen-Bonded Frameworks for Anion Binding and Separation", *American Crystallographic Association Meeting, Supramolecular Chemistry Symposium*, July 25, **2007**, Salt Lake City, invited presentation.
 25. Custelcean, R. "Strategies for the Design of Crystalline Organic Materials", *Organic Magnetism Symposium*, Oak Ridge Natl. Lab., July 16-17, **2007**, invited presentation.
 24. Custelcean, R.; Moyer, B. A.; Hay, B. P., Bonnesen, P. V.; Delmau, L. H. "Anion Coordination and Separation with Metal-Organic and Hydrogen-Bonded Frameworks", *DOE Contractors' Meeting*, April 24-27, **2007**, Annapolis, MD, poster presentation.
 23. Custelcean, R.; Moyer, B. A.; Gorbunova, M. G.; Hay, B. P. "Anion Coordination and Separation with Metal-Organic Frameworks", *American Chemical Society Meeting*, March 26-30, **2006**, Atlanta, oral presentation.
 22. Custelcean, R.; Gorbunova, M. G.; Bonnesen, P. V.; Hay, B. P.; Moyer, B. A. "Anion Recognition and Separation with Metal-Organic Frameworks", *Pacificchem 05*, Dec 16-20, **2005**, Honolulu, Hawaii, oral presentation.
 21. Custelcean, R.; Gorbunova, M. G.; Bonnesen, P. V.; Hay, B. P.; Moyer, B. A. "Towards Anion Recognition and Separation in Metal-Organic Frameworks", *American Crystallographic Association Annual Meeting, Crystal Engineering Symposium*, May 28-June 2, **2005**, Orlando FL, invited presentation.
 20. Custelcean, R.; Gorbunova, M. G.; Moyer, B. A.; Bonnesen, P. V.; Delmau L. H.; Hay, B. P. "Principles of Chemical Recognition and Transport in Extractive Separations: Metal-Organic Frameworks as Solid-Phase Anion Exchangers", *DOE Contractors' Meeting*, April 27-30, **2005**, Rockville, MD, invited presentation.
 19. Custelcean, R.; Dreger, Z. A. "Dihydrogen Bonding under High Pressure: A Raman Study of BH₃NH₃ molecular crystal", *13th American Physical Society Topical Conference on Shock Compression of Condensed Matter*, July 20-25, **2003**, Portland, Oregon, oral presentation.
 18. Custelcean, R.; Dreger, Z. A. "Dihydrogen Bonding under High Pressure" *Midwest Organic*

- Solid State Chemistry Symposium*, June 6-7, **2003**, University of Minnesota, Minneapolis, poster presentation.
17. Custelcean, R. "Crystal Design via Conventional and Unconventional Hydrogen Bonding", March **2003**, Howard University, invited presentation.
 16. Custelcean, R. "Crystal Design via Conventional and Unconventional Hydrogen Bonding", March **2003**, University of Nevada at Las Vegas, invited presentation.
 15. Custelcean, R. "Crystal Design via Conventional and Unconventional Hydrogen Bonding", March **2003**, Oak Ridge National Laboratory, invited presentation.
 14. Custelcean, R. "Crystal Design via Conventional and Unconventional Hydrogen Bonding", February **2003**, Central Michigan University, invited presentation.
 13. Custelcean, R. "Crystal Design via Conventional and Unconventional Hydrogen Bonding", January **2003**, George Washington University, invited presentation.
 12. Custelcean, R. "Rational Assembly of Molecular and Covalent Materials using Conventional and Unconventional Hydrogen Bonding", February **2002**, University of Alberta, invited presentation.
 11. Custelcean, R. "Rational Assembly of Molecular and Covalent Materials using Conventional and Unconventional Hydrogen Bonding", February **2002**, University of Toledo, invited presentation.
 10. Custelcean, R. "Rational Assembly of Covalent Materials via Dihydrogen Bonding", February **2002**, Washington State University, invited presentation.
 9. Custelcean, R.; Ward, M. D. "Chiral Organization in Hydrogen-Bonded Crystals" *Industrial Partnership for Research in Interfacial and Materials Engineering Conference*, May 28-31, **2002**, University of Minnesota, Minneapolis, oral presentation.
 8. Custelcean, R. "Rational Assembly of Covalent Materials via Dihydrogen Bonding", **2001**, Pfizer, Groton, Connecticut, invited presentation.
 7. Custelcean, R., Ward, M. D. "Supramolecular Chirality in Porous Hydrogen-Bonded Networks" *Midwest Organic Solid State Chemistry Symposium*, June 8-9, **2001**, Nebraska, Lincoln, oral presentation.
 6. Custelcean, R., Ward, M. D. "Supramolecular Organization in Chiral Guanidinium Sulfonates" *Industrial Partnership for Research in Interfacial and Materials Engineering Conference*, May 5-7, **2001**, University of Minnesota, Minneapolis, oral presentation.
 5. Custelcean, R., Jackson, J. E. "Toward Crystalline Covalent Solids: Crystal-to-Crystal Dihydrogen to Covalent Bonding Transformation in NaBH₄·THEC" *Gordon Research Conference: Organic Structures and Properties*, June 17-22, **2000**, Connecticut College, New London, Connecticut, poster presentation.
 4. Custelcean, R., Jackson, J. E. "Toward Extended Crystalline Solids: Topotactic Dihydrogen to Covalent Bonding Transformation in NaBH₄·THEC" *Center for Fundamental Materials Research Symposium*, February 27-28, **2000**, Michigan State University, East Lansing, poster presentation.
 3. Custelcean, R., Jackson, J. E. "Structure and Topochemical Decomposition of a Dihydrogen-Bonded System with Exceptionally Short H···H Distances and Enhanced Solid State Reactivity" *Center for Fundamental Materials Research Symposium*, March 14-15, **1999**, Michigan State University, East Lansing, poster presentation.
 2. Custelcean, R., Jackson, J. E. "Hydrogen-Hydrogen Hydrogen Bonds as Chemical Basting Stitches" *American Chemical Society National Meeting*, August 23-27, **1998**, Boston, Massachusetts, poster presentation.

1. Custelcean, R., Jackson, J. E. "Hydrogen-Hydrogen Hydrogen Bonds as Chemical Basting Stitches", *Center for Fundamental Materials Research Symposium*, March 1-2, **1998**, Michigan State University, East Lansing, poster presentation.