Curriculum Vitae

Radu Custelcean

Research Scientist, Oak Ridge National Laboratory
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Education

2000 Ph.D. Chemistry, Michigan State University (with James E. Jackson)
"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

2003-present Research Scientist, Oak Ridge National Laboratory
crystalline materials for energy and environmental applications; supramolecular chemistry; crystal engineering; chemical separations; anion receptors; 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 (with Mike Ward)
crystal engineering; solid-state organic chemistry; hydrogen-bonded materials

Research Interests: self-assembled structures for environmental and energy applications; supramolecular chemistry; crystal engineering; chemical separations; anion recognition.

Recognitions, Honors, Awards

- *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)

- 9 papers featured on journal covers: *Angew. Chem.* (2015, 2005), *ChemComm* (2013, 2012, 2005), *Cryst. Growth Des.* (2009, 2008), *Eur. J. Inorg. Chem.* (2007), *Struct. Chem.* (1999).

- *Angew. Chem.* paper highlighted in *Chemistry World*, April 27, 2009
- *ChemComm* paper highlighted on the ACS webpage (January 23, 2006)

Professional Activities and Memberships

- Member of the editorial board for *Journal of Crystallography*, 2012-present
- 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
- Member of the American Chemical Society
- Member of the American Crystallographic Association

Teaching and Mentoring

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

2003-present: supervised 5 postdocs, 6 master students, and 2 undergraduate students

Funding

External

DOE-BES, 10/2014–9/2016; *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, 10/2011–09/2013; *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:

87. 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 cover).
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 CO_2 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 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 M_4L_6 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: CeX_3·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 $(Ba,Sr)_{4-x}La_{2x}Co_4O_{15}$", 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 $TlFe_{1.6}Se_2$ 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 = Ca, Eu, 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 YbMg2Bi2," 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 $CeCl_3(CH_3OH)_4$*", *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 2Dioxane·$2H_2O$·$CuCl_2$: 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.; Kolupus, J. A.; Chakoumakos, B. C.; Wisniewska, M.; Custelcean, R. "*Single-Crystal CeCl3(CH3OH)4: A new metal-organic cerium chloride methanol aduct 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'-Binicotinic 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.
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18. Custelcean, R.; Dreger, Z. A. "Dihydrogen Bonding under High Pressure: A Raman Study of BH_3NH_3 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 $NaBH_4$·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 $NaBH_4$·THEC" *Angew. Chem. Int. Ed.* **2000**, *39*, 3299.
11. Custelcean, R.; Jackson, J. E. "Topochemical Dihydrogen to Covalent Bonding Transformation in $LiBH_4$·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 BH_4CN and BH_5" *J. Mol. Struct. Theochem* **2000**, *505*, 95.
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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(*3H*)-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:

Custelcean, R.; Moyer, B. A.; Rajbanshi, A. "Selective Oxoanion Separation Using a Tripodal Ligand" US20130319950 A1, **2013**.

Presentations:

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", *Pacifichem* **2010**, Hawaii, invited presentation.
35. Custelcean, R. "Anion Recognition and Separation with Self-Assembled Cage Receptors", *Pacifichem* **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", *Pacifichem 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 BH_3NH_3 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 $NaBH_4$·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 $NaBH_4$·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.