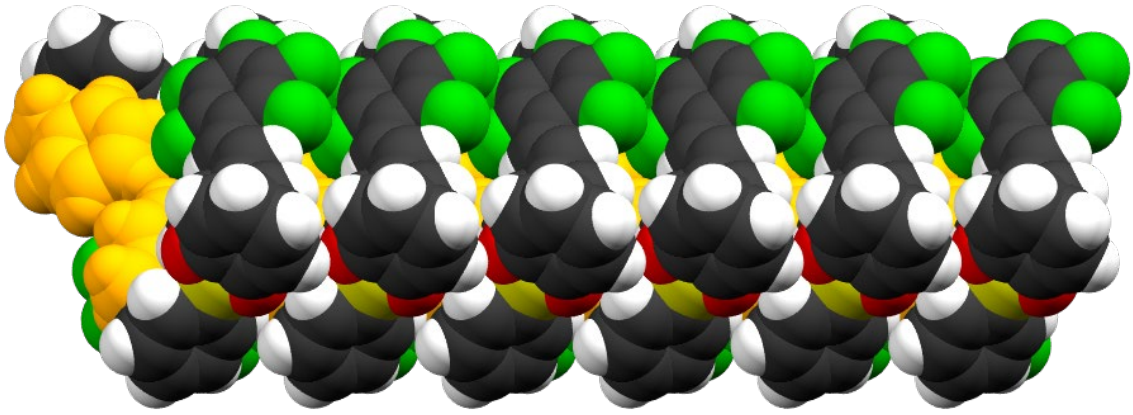
Virtual Midwest Organic Solid-State Chemistry Symposium (V-MOSSCS)



https://mosscs2021.web.illinois.edu/

June 18th, 2021

University of Iowa

Iowa City, Iowa

Sponsors:

The financial support of the following sponsors is gratefully acknowledged:

Organizing Committee

Prof. Len MacGillivray – University of Iowa

Prof. Lewis Stevens – University of Iowa

Prof. Alexei V. Tivanski – University of Iowa

Dr. Gonzalo Campillo-Alvarado – University of Illinois at Urbana-Champaign

Midwest Organic Solid-State Chemistry Symposium

MOSSCS is a gathering that provides students, postdoctoral fellows, and faculty an excellent opportunity to present research on the organic solid state in an informal setting. The first MOSSCS was held in 1988 at the University of Illinois-Urbana Champaign (UIUC). Subsequent meetings have continued to welcome participants from a national base of academic and industrial institutions. With efforts to manage effects of the COVID-19 pandemic and provide opportunities to share information on the organic solid state, MOSSCS is being held virtually for 2021 as V-MOSSCS. The charter of the symposium is to provide an opportunity to exchange ideas and research results in an informal atmosphere, with the main emphasis being on presentations by graduate and undergraduate students. The meetings have been rotated among academic and industrial sites in the Midwest of the United States.

V-MOSSCS – GENERAL PROGRAM

Friday, June 18th, 2021

08:00 – 08:15	Welcome to Symposium and Opening Remarks
08:15 – 10:00	Scientific Session I
10:00 – 10:15	Break
10:15 – 12:00	Scientific Session II
12:00 – 13:30	Lunch & Poster Session (Gather Town)
13:30 – 14:45	Scientific Session III
14:45 – 15:00	Break
15:00 – 15:45	Scientific Session IV
16:00 – 16:10	Final remarks
16:10 – 16:30	Break
16:30 – 18:00	Social Hour, Awards and Poster Gallery (Gather Town)

V-MOSSCS – PROGRAM

Friday, June 18th

8:00 **Welcome and Opening Remarks**

Scientific Session I *– Travis Holman, Presiding*

8:15 **S1-1 KEYNOTE LECTURE:** *Jonathan W. Steed*, Department of Chemistry, Durham University, Durham, UK, **Gel Based Approaches to the Polymorph Landscape**

8:45 **S1-2** *Rahul K. Shahni, Micah Mabin, Zhihan Wang, Muneer Shaik, Angel Ugrinov, and Qianli R. Chu,* Department of Chemistry, University of North Dakota, Grand Forks ND, **Synthesis and Characterization of BPA-free Polyesters by Incorporating a Semi-rigid Cyclobutanediol Monomer**

9:00 **S1-3** *Beth A. Young and Lewis L. Stevens,* Department of Pharmaceutical Sciences and Experimental Therapeutics, University of Iowa, College of Pharmacy, Iowa City, IA, **Discriminating the interaction anisotropy in polymorphs using powder Brillouin light scattering**

9:15 **S1-4** *Daniel Davies and Ying Diao,* Department of Chemical and Biomolecular Engineering, University of Illinois, Urbana-Champaign, Urbana, IL, **Controlling Polymorphic Phase Transitions Via Alkyl Chain Engineering**

9:30 **S1-5** *Joseph Robertson and Q. Rick Chu,* Department of Chemistry, University of North Dakota, Grand Forks, ND, **Rigidity Calculator: A Tool for the Quantification of Rigidity of Small Molecules**

9:45 **S1-6** *Manish Kumar Mishra,* Vellore Institute of Technology, Vellore, Tamil Nadu, India, **Crystal Engineering with ionic liquids**

10:00 **V-MOSSCS Group Photo and Break** (15 min)

Scientific Session II *– Alexei V. Tivanski, Presiding*

10:15 **S2-1 KEYNOTE LECTURE:** *Kristin M. Hutchins*, Texas Tech University, Department of Chemistry and Biochemistry, Lubbock, TX, USA, **Influence of Crystal Packing and Molecular Motion on Thermal Expansion in Organic Solids**

10:45 **S2-2** *Vinu V. Panikkattu, Abhijeet S. Sinha, Boris Averkiev, Christer B. Aakeröy* Department of Chemistry, Kansas State University, **Structural and theoretical analysis of 'triply activated' molecules with exceptional σ-hole values**

11:00 **S2-3** *Christopher J. Hartwick, Shweta P. Yelgaonkar, Eric W. Reinheimer, Gonzalo Campillo-Alvarado, Leonard R. MacGillivray** Department of Chemistry, University of Iowa, Iowa City, IA, **B-N Self-assembly: U-shaped bipyridine diboron complexes**

11:15 **S2-4** *Kelly N. Shunje,[a] Ruwandi Kumarasinghe,[b] Ganga M. Hettiarachchi,[b] and Christer B. Aakeröy,[a]* [a]Department of Chemistry, Kansas State University,Manhattan, KS, [b]Department of Agronomy, Kansas State University, Manhattan, KS, **Enhancing the Physicochemical Properties of Agrochemicals Using CrystalEngineering**

11:30 **S2-5** *Andrew Kelly, K. Travis Holman,* Georgetown University, **"Click"-Like η 6 - Metalation/Demetalation of Simple Aryl Halides as a Means of Turning "ON/OFF" Halogen Bond**

11:45 **S2-6** *Viraj De Silva, Boris Averkiev, Abhijeet Sinha, Christer B. Aakeröy,* Department of Chemistry, Kansas State University, Manhattan, KS, **Cause and effect: Fine tuning σ-hole potentials for controlling the balance between intermolecular interactions**

12:00 **Poster Session and Lunch (90 min.)**

Scientific Session III *– Lewis Stevens, Presiding*

13:30 **S3-1 KEYNOTE LECTURE:** *Calvin Sun*, Department of Pharmaceutics, University of Minnesota, Minneapolis, MN, **Enabling tablet developmentthrough crystal engineering**

14:00 **S3-2** *Michael Bernhardt, Gonzalo Campillo-Alvarado, and Ying Diao,* Department of Chemical and Biomolecular Engineering, University of Illinois Urbana- Champaign, Urbana, IL, **Selection of π-stacking modes of an organic semiconductor via cocrystallization**

14:15 **S3-3** *Shankar Gairhe, Anjaneyulu Putta and Haoran Sun,* Department of Chemistry, Center for fluorinated functional materials, University of South Dakota, Vermillion, SD, **Crystal structures of methoxy substituted perfluorobutylated tetrabenzo[a,c,h,j]phenazines**

14:30 **S3-4** *María G. Vasquez-Ríos, Gonzalo Campillo-Alvarado and Leonard R. MacGillivray,* Department of Chemistry, University of Iowa, Iowa City, 1A, **Supramolecular Assemblies of Diboronic Acids and Bipyridines Involving Polymers and, Crystal-to-Crystal [2 + 2] Photodimerization in the Solid State**

14:45 **Break** (15 min)

Scientific Session IV *– Gonzalo Campillo-Alvarado, Presiding*

15:00 **S4-1** *Ryan H. Groeneman,[a] Michael A. Sinnwell,[b] and Leonard R. MacGillivray,[a]* [a]Department of Biological Sciences, Webster University, St. Louis, Missouri, [b]Department of Chemistry, University of Iowa, Iowa City, Iowa, **Engineering cross-photoreactions in the organic solid state**

15:15 **S4-2** *Daniel Padeanu, David Evans, George Shimizu,* University of Calgary, **Modifying Pore Structure in Chromium-Phosphonate MOFs through Selective Templating**

15:30 **S4-3** *Yuze Zhang,[a,b] Alexander G. Shtukenberg,[b] Dilhan M. Kalyon,[a] Bart Kahr,[b] Stephanie S. Lee,[b]* [a]Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ, [b]Molecular Design Institute, Department of Chemistry, New York University, New York, NY, **Role of Melt Phase Properties and Conditions on the Twisting Behavior of Mannitol Crystals**

15:45 **S4-4** *Marie E. Fiori,*[a] *Kushal Bagchi1,[a] Michael F. Toney,[b] M. D. Ediger,[a]* [a]Department of Chemistry, University of Wisconsin-Madison, Madison, WI, [b]Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO, **Controlling PVD glass structure near organic-organic interfaces**

16:00 **Final Remarks**

16:10 – 16:30 Short break

16:30 **Awards, Social Hour and Poster Gallery** *– See you in Gather Town!* (90 min)

Poster Presentations (June 18th, 12:00 – 13:30)

P1. *Gerrit Vreeman, Manish Mishra, Changquan Calvin Sun,* Department of Pharmaceutics, University of Minnesota Twin Cities, Minneapolis, MN, 55455, **Improved tabletability upon salt formation despite reduced plasticity**

P2. *Zijian Wang,[a] Chenguang Wang,[a] Cheng Liang,[b] Imanuel Bier,[c] Changquan Calvin Sun,[a]* [a]Department of Pharmaceutics, University of Minnesota Twin Cities, Minneapolis, MN, [b]Technical Development, Biogen, Cambridge, MA, [c]Dept. of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA. **The relationships among the crystal structure, mechanical properties, surface energy, and tabletability investigated with p-aminobenzoic acid polymorphs**

P3. *Xiaodan Ding,[a] Daniel K. Unruh,[a] Ryan H. Groeneman,[b] and Kristin M. Hutchins,[a]* [a]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas. [b]Department of Biological Sciences, Webster University, St. Louis, Missouri. **Thermal Expansion Behaviors of Unique Solids: Mixed Cocrystals and Stoichiometric Polymorphs of Traditional Cocrystals**

P4. *Taylor J. Dunning,[a] Carlos L. Santana,[a] Eric Bosch[b] and Ryan H. Groeneman*,[a] [a]Webster University, Department of Biological Sciences, St. Louis, Missouri, [b]Department of Chemistry, Missouri State University, Springfield, Missouri. **Halogen-bonded networks based upon nodes generated from the [2 + 2] cycloaddition reaction**

P5. *Gary C. George III*, *Daniel K. Unruh, and Kristin M. Hutchins*, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX. **Modifying Thermal Expansion Properties of Organic Solids via Cycloaddition Reactions**

P6. *Giselle Lin,[a] George K. H. Shimizu*, [a]Department of Chemistry, University of Calgary [a]Department of Biological Sciences, Calgary, Canada. **Investigating High-Temperature Proton Conduction via Guest-Loaded Metal-Organic Frameworks**

P7. *Giselle Lin,[a] Valerie Brunskill, Garima Lal, Shiron Lee, and George Shimizu*, [a]Department of Chemistry, University of Calgary [a]Department of Biological Sciences, Calgary, Canada. **Self-assembly behaviour of amphiphilic metal organic polyhedra**

P8. *Bronwyn G. Metcalf, Dr. Jay WM. Wackerly*, Central College, Pella, IA. **Synthesis and host-guest binding of cambiarene macrocycles**

P9. *Qixuan Zheng, Daniel K. Unruh, and Kristin M. Hutchins*, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas. **Cocrystallization of Trimethoprim and Solubility Enhancement via Salt Formation**

P10. *Jesus Daniel Loya, Daniel K. Unruh, and Kristin M. Hutchins*, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX. **Co-crystallization of the Herbicide 2,4-D**

P11. *Al Tiba, Leonard R. MacGillivray, Alexei Tivanski,* Department of Chemistry, University of Iowa, Iowa City, IA. **Mechanical properties of a shape-memory metal-organic framework: [Cu2(bdc)2(bpy)]n (bdc = 1,4-benzenedicarboxylate, bpy = 4,4'-bipyridine)**

P12. *Dherya Bahl and Lewis L. Stevens*, Department of Pharmaceutical Sciences and Experimental Therapeutics, University of Iowa, College of Pharmacy, Iowa City, IA. **Manipulating cocrystal stoichiometry to improve solubility**

P13. *Celymar Ortiz de Leon and Leonard R. MacGillivray*, Department of Chemistry, University of Iowa, Iowa City, IA. **Ternary cocrystals, noncovalent bridges and supramolecular isomerism**