Nanoporous Materials & Their Applications

Gordon Research Conference

Established Materials and Emerging Opportunities

August 9-14, 2015 Holderness School Holderness, NH

Chair: David Sholl Vice Chair: Guang Cao

Contributors



















Meeting Program

Sunday 2:00 pm - 9:00 pm Arrival and Check-in 6:00 pm Dinner 7:30 pm - 7:40 pm Welcome / Introductory Comments by GRC Site Staff 7:40 pm - 9:30 pm **New Synthesis Strategies for Nanoporous Materials** Discussion Leader: Alexandra Navrotsky (University of California, Davis, USA) Enrique Iglesia (University of California, Berkeley, USA) 7:40 pm - 8:20 pm "Strategies for the Synthesis of Zeolites and for the Encapsulation of Clusters Within Their Voids" 8:20 pm - 8:35 pm Discussion

8:35 pm - 9:15 pm	Mike Zawarotko (University of Limerick, Ireland) "Crystal Engineering of Hybrid Porous Materials"		
9:15 pm - 9:30 pm	Discussion		
Monday			
7:30 am - 8:30 am	Breakfast		
8:30 am	Group Photo		
9:00 am - 12:30 pm	Materials for Emerging Applications		
	Discussion Leader: Omar Farha (Northwestern University, USA)		
9:00 am - 9:40 am	Paul Webley (University of Melbourne, Australia) "Advanced Materials for Highly Selective Carbon Dioxide Capture"		
9:40 am - 10:00 am	Discussion		
10:00 am - 10:30 am	Coffee Break		
10:30 am - 11:10 am	Freek Kapteijn (Delft University of Technology, The Netherlands) "Adsorptive Heat Pumps: Can MOFs Replace Existing Sorbents?"		
11:10 am - 11:30 am	Discussion		
11:30 am - 12:10 pm	Ryan Lively (Georgia Institute of Technology, USA) "Impact of Zeolitic Imidazolate Framework Flexibility on Molecular Separation Processes"		
12:10 pm - 12:30 pm	Discussion		
12:30 pm	Lunch		
1:30 pm - 4:00 pm	Free Time		
4:00 pm - 6:00 pm	Poster Session		
6:00 pm	Dinner		
7:30 pm - 9:30 pm	New Materials for Catalysis		
	Discussion Leader: Krista Walton (Georgia Institute of Technology, USA)		
7:30 pm - 8:10 pm	Laura Gagliardi (University of Minnesota, USA) "Metal-Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts"		
8:10 pm - 8:30 pm	Discussion		
8:30 pm - 9:10 pm	Christian Doonan (The University of Adelaide, Australia) "Following Chemical Reactions in MOF Pores"		
9:10 pm - 9:30 pm	Discussion		

Tuesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Enhancing Zeolite Properties via Synthesis and Modeling
	Discussion Leader: Georgi Vayssilov (University of Sofia, Faculty of Chemistry and Pharmacy, Bulgaria)
9:00 am - 9:40 am	Alex Katz (University of California, Berkeley, USA) "Functional Nanopores in Carbonaceous and Zeolitic Catalysts"
9:40 am - 10:00 am	Discussion
10:00 am - 10:30 am	Coffee Break
10:30 am - 11:10 am	Preeti Kamakoti (ExxonMobil Research and Engineering, USA) "Modeling Adsorption in Cationic Zeolites: Trials and Tribulations"
11:10 am - 11:30 am	Discussion
11:30 am - 12:10 pm	Christine Kirschhock (KU Leuven, Belgium) "Zeolite Synthesis: A Lego Game?"
12:10 pm - 12:30 pm	Discussion
12:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm	Dinner
7:30 pm - 9:30 pm	Unconventional Synthesis Methods
	Discussion Leader: Russell Morris (University of St. Andrews, United Kingdom)
7:30 pm - 8:10 pm	Feng-Shou Xiao (Zhejiang University, China) "Sustainable Synthesis of Zeolites and Stability Enhancement of Porous Organic Materials"
8:10 pm - 8:30 pm	Discussion
8:30 pm - 9:10 pm	Tomislav Friscic (McGill University, Canada) "Mechanochemistry: Resolving the Challenges of Bulk Synthesis of Metal-Organic Frameworks"
9:10 pm - 9:30 pm	Discussion

	Wednesday			
,	7:30 am - 8:30 am	Breakfast		
9:00 am - 12:30 pm		Conductive MOFs		
		Discussion Leader: Phillip Llewellyn (Aix-Marseille University, France)		
	9:00 am - 9:40 am	Mircea Dinca (Massachusetts Institute of Technology, USA) "Enabling and Utilizing Charge Transport in Microporous Metal-Organic Frameworks"		
	9:40 am - 10:00 am	Discussion		
	10:00 am - 10:30 am	Coffee Break		
	10:30 am - 11:10 am	Deanna D'Allessandro (University of Sydney, Australia) "A Combined Experimental, Theoretical and Computational Approach to Redox-Active Microporous Materials"		
	11:10 am - 11:30 am	Discussion		
11:30 am - 12:10 pm Satoshi Horike (Kyoto University, Japan) "Development of Ion Conductive, Glassy, and Melting MOFs with Poro		Satoshi Horike (Kyoto University, Japan) "Development of Ion Conductive, Glassy, and Melting MOFs with Porosity"		
	12:10 pm - 12:30 pm	Discussion		
12:30 pm Lunch		Lunch		
1:30 pm - 4:00 pm Free Time		Free Time		
4:00 pm - 6:00 pm Poster Session		Poster Session		
	6:00 pm	Dinner		
	7:00 pm - 7:30 pm	Business Meeting		
		Nominations for the Next Vice Chair; Fill in Conference Evaluation Forms; Discuss Future Site and Scheduling Preferences; Election of the Next Vice Chair		
	7:30 pm - 9:30 pm	New Frontiers for MOFs		
		Discussion Leader: Kim Jelfs (Imperial College London, United Kingdom)		
	7:30 pm - 8:10 pm	Norbert Stock (Christian-Albrechts University of Kiel, Germany) "Al-Based Metal-Organic Frameworks: From High-Throughput Investigations to Continuous Flow Synthesis"		
	8:10 pm - 8:30 pm	Discussion		
	8:30 pm - 9:10 pm	Seth Cohen (University of California, San Diego, USA) "The MOF-Polymer Interface: Top-Down and Bottom-Up Approaches"		
	9:10 pm - 9:30 pm	Discussion		

Thursday				
7:30 am - 8:30 am	Breakfast			
9:00 am - 12:30 pm	New Frontiers in Synthesis and Characterization			
	Discussion Leader: Minkee Choi (Korea Advanced Institute of Science & Technology, South Korea)			
9:00 am - 9:40 am	Matthias Thommes (Quantachrome, USA) "Advances in the Textural Characterization of Nanoporous Materials with Hierarchical Pore Structure"			
9:40 am - 10:00 am	Discussion			
10:00 am - 10:30 am	Coffee Break			
10:30 am - 11:10 am	Scott Auerbach (University of Massachusetts, Amherst, USA) "Sipping from the Holy Grail: Modeling the Molecular Formation of Ordered Nanoporous Materials"			
11:10 am - 11:30 am	Discussion			
11:30 am - 12:10 pm Jeffrey Rimer (University of Houston, USA) "Elements of Rational Design: New Approaches to Tailor Zeolite Crys				
12:10 pm - 12:30 pm	Discussion			
12:30 pm	Lunch			
1:30 pm - 4:00 pm	Free Time			
4:00 pm - 6:00 pm	Poster Session			
6:00 pm	Dinner			
7:30 pm - 9:30 pm	Catalysis and Separations			
	Discussion Leader: Chia-Kuang Tsung (Boston College, USA)			
7:30 pm - 8:10 pm	Praveen K. Thallapally (Pacific Northwest National Laboratory, USA) "Metal Organic Frameworks for Xenon and Krypton Separation Applications"			
8:10 pm - 8:30 pm	Discussion			
8:30 pm - 9:30 pm	Short Talks Selected from Poster Abstracts			
Friday				
7:30 am - 8:30 am	Breakfast			
9:00 am	Departure			

Poster List

Display your poster at the board # and session indicated below. If your name does not appear in the list, display your poster at the next available board in the session which seems most appropriate, or consult with the conference chairs about which session to present in. There is plenty of space available for additional posters.

Poster Session I (Monday/Tuesday)

#	Name	Organization	Co-Authors	Poster Title
1	Agrawal, Kumar Varoon	Massachusetts Institute of Technology	Steven Shimizu, Michael Strano	Experimental investigation of phase transition of water inside carbon nanotube nanopore
2	Arab, Pezhman	Virginia Commonwealth university	Ali R. Siamaki, Frank Gupton, and Hani M. El- Kaderi	Synthesis of a Pd(II)- Functionalized Mesoporous Covalent Organic Framework as a Heterogeneous Catalyst for Suzuki Reaction
3	Barin, Gokhan	University of California, Berkeley	Gregory W. Peterson, Jeffrey R. Long	High Capacity Porous Organic Polymers for Ammonia Capture
4	Brand, Stephen K	California Institute of Technology	Jay A. Labinger, Mark E. Davis	Tin Silsesquioxane Complexes as Models for the Proposed Active Sites in Sn-Beta
5	Burtch, Nicholas C	Georgia Institute of Technology	Nicholas Burtch, Krista Walton	Tools for Exploring Hydrothermal Stability Mechanisms in Metal- Organic Frameworks
6	Chiang, Wei-Shan	National Institute of Standards and Technology	Emiliano Fratini, Piero Baglioni, Daniel Georgi, Jinhong Chen, and Yun Liu	Methane Adsorption in Model Porous Material SBA-15 Studied by Small-Angle Neutron Scattering
7	Chou, Lien-Yang	Boston College	Allison Young, and Chia- Kuang (Frank) Tsung*	Metal Nanoparticles Synthesis using Metal Organic Framework as Crystalline Capping Agent and their Catalytic Properties
8	Egodawatte, Shani N	University of Iowa	Ashish Datt, Katherine E.Greenstein, David M. Cwiertny, Sarah C. Larsen	Adsorption of Environmental Contaminants on Iron Oxide/ Mesoporous Silica Core Shell Nanomaterials
9	Fernandez, Laura E	University of Minnesota	Rachel Klet, § Timothy Wang, § Donald G. Truhlar,* Omar Farha, § and Joseph Hupp§	Atomic layer deposition (ALD) of zinc on zirconium metal–organic frameworks (MOFs)
10	Gee, Jason	Georgia Institute of Technology		Computational Identification and Experimental Evaluation of Metal-Organic Frameworks for Xylene Enrichment
11	Holden, Daniel	University of Liverpool	Kim Jelfs, Maciek Haranczyk, Andrew Cooper	Gas Diffusion in a Porous Organic Cage: Analysis of Dynamic Pore Connectivity using Molecular Dynamics Simulations

12 Iida, Takayuki	The University of Tokyo	Prof. Tatsuya Okubo, Prof. Toru Wakihara	Unique features of the efficient preparation of Sn-beta zeolites from Sn-Si mixed oxide composites
13 Jayachandrababu, Krishna C	Georgia Institute of Technology	Ross J. Verploegh, David S. Sholl, Sankar Nair	Structure and Tunable Properties of Hybrid Zeolitic Imidazolate Frameworks
14 Jeon, Mi Young	University of Minnesota	Donghun Kim, Prashant Kumar, Pyung-Soo Lee, and Michael Tsapatsis	Bottom-up synthesis of single MFI nanosheets via seeded growth and their membrane applications
15 Khan, Mohammad Navaid	University of Massachusetts Amherst	Scott M. Auerbach, Peter A. Monson	Study of the Effects of Structure Directing Agents on the Self- Assembly Process of Ordered Microporous Materials
16 Khare, Rachit	University of Minnesota	Dean Millar, Aditya Bhan	Methanol-to-hydrocarbons conversion: Effects of crystallite size and intrinsic mechanistic behavior of MFI
17 Kim, Kyoungsoo	Institute for Basic Science, KAIST	Younjae Jung, Minkee Choi, Ryong Ryoo*	Templating Synthesis of hierarchically porous carbon via steam-assisted carbonization in nanocrystalline beta zeolite for high-rate electrical double layer capacitor
18 Koller, Hubert	University of Muenster		Advanced H-Al Distance Analyses in Zeolite Acid Sites by Solid State NMR
19 Kumar, Manjesh	University of Houston	Jeffrey D. Rimer	Identifying the Mechanism of SSZ- 13 Crystallization and Methods to Tailor Material Properties
20 Lapidus, Saul H	Argonne National Laboratory		TBD
21 Lee, Munhee	Institute for Basic Science (KAIST) campus center)	Yongbeom Seo, Changbum Jo, Hyesun Shin, and Ryong Ryoo*	Two unit-cell thick anatase titania nanosheets with mainly exposed (010) high-energy facet
22 Lippi, Renata	University of Adelaide & Commonwealth Scientific and Industrial Research Organisation (CSIRO)	Campbell J. Coghlan, Matthew R. Hill, Christopher J. Sumby, Christian J. Doonan and Danielle F. Kennedy	Postsynthetic metallated MOF a pre-catalyst for gas phase CO2 reduction
23 Luo, Helen Y	Massachusetts Institute of Technology	Vladimir K. Michaelis, Sydney Hodges, Robert G. Griffin, Yuriy Roman-Leshkov	One-pot synthesis of MWW zeolite nansoheets using a rationally designed organic structuredirecting agent
24 Marti, Anne M	The National Energy and Technology Laboratory	Jeff Culp, Surendar Venna, David Hopkinson	Metal Organic Framework Materials for CO2 Capture

25 Milina, Maria	Massachusetts Institute of Technology	Sharon Mitchell, David Cooke, Paolo Crivelli, and Javier Pérez-Ramírez	Impact of Pore Connectivity on the Design of Long-Lived Zeolite Catalysts
26 Morabito, Joseph V	Boston College	Chia-Kuang Tsung	Kinetic Studies of Bridging Ligand Exchange in Metal-Organic Frameworks
27 Mounfield, William P	Georgia Institute of Technology	U. Tumuluri, Y. Jiao, Z. Wu, K.S. Walton	In Situ IR Spectroscopic Investigation of Acid Gas Adsorption on MOF-derived Ceria
28 Oleksiak, Matthew D	University of Houston	Marlon T. Conato, Jeffrey D. Rimer	Tailoring the physicochemical properties of zeolites via organic structure-directing agent free synthesis routes
29 Pilyugina, Tatiana S	Aramco Research Center - Boston	Sarah L. Kobaslija, Sergio Fernandez	Hard- and soft-templated syntheses as well as template-free steam-assisted dry gel conversion as methods for preparation of mesoporous zeolite Beta.
30 Rangnekar, Neel	University of Minnesota	Meera Shete, Kumar Varoon Agrawal, Berna Topuz, Prashant Kumar, Qiang Guo, Issam Ismail, Benjamin Stottrup, Michael Tsapatsis	Monolayer deposition and secondary growth of 3 nm-thick 2D zeolites
31 Ravikovitch, Peter	Exxonmobil Research and Engineering		TBD
32 Seo, Dong-Kyun	Arizona State University	Dinesh Medpelli, Danielle M. Ladd, Farid Akhtar	Exceptional Carbon Dioxide Sorption Properties of Hierarchical FAU Zeolites Having a High Crystallinity
33 Snyder, Mark A	Lehigh University	Zheng Tian, Shih-Chieh Kung, Daniel G. Gregory, Qianying Guo, Megha Sharma, Mark A. Snyder	Template-Mediated Multiscale Structuring of Crystalline and Amorphous Porous Materials
34 Van Der Mynsbrugge, Jeroen	Ghent University	Jeroen Van der Mynsbrugge, Kristof De Wispelaere, Pieter Cnudde and Veronique Van Speybroeck	Toward a more accurate computational description of adsorption in Brønsted acid zeolites
35 Vargas, Ernesto	Northwestern University	Randall Q. Snurr	Anisotropic, heterogeneous diffusion in the metal-organic framework NU-1000
36 Verploegh, Ross J	Georgia Institute of Technology	Sankar Nair, David S. Sholl	Temperature and Loading- Dependent Diffusion of Light Hydrocarbons in Zeolitic Imidazolate Framework-8 as Predicted Through Fully Flexible Molecular Simulations
37 Walton, Ian	University at Buffalo, SUNY	Jordan M. Cox, Jason B. Benedict	Light-responsive MOFs: Functionalization of metal-organic frameworks through the design and synthesis of photochromic linkers.

38 Yan, Yushan	University of Delaware	Qianrong Fang and Shilun Qiu	Covalent organic frameworks (COFs): From design to applications
39 Zhang, Han	University of Minnesota	Michael Tsapatsis, Chris Macosko	Mild Detemplation of Sub-Micro Silicalite-1 Membranes for Xylene and Butane Isomer Separation

Poster Session II (Wednesday/Thursday)

#	Name	Organization	Co-Authors	Poster Title
1	Akimbekov, Zamirbek	Peter A. Rock Thermochemistry Laboratory, University of California, Davis		TBD
2	Aubrey, Michael L	University of California, Berkeley	Jeffrey R. Long	Oxidative Insertion of Weakly Coordinating Anions in a Metal- Organic Framework
3	Benedict, Jason B	University at Buffalo		Please see below
4	Brown, Craig M	NIST Center for Neutron Research	Craig M. Brown	Neutron and X-ray scattering of adsorbates nanoporous materials
5	Chapman, Karena W	Argonne National Laboratory		Probing structural disorder in framework materials
6	Chien, Szu-Chia	UMASS-Amherst	Scott Auerbach, Peter Monson	Modeling the Self-Assembly of Silica Microporous Materials
7	Choi, Minkee	Korea Advanced Institute of Science & Technology	Chang Hyuck Choi, Minho Kim, Han Chang Kwon,, Karl J. J. Mayrhofer, Hyungjun Kim, and Minkee Choi*	Oxygen Reduction by Single-Atom Pt: Selective Production of H2O2 instead of H2O
8	Cockayne, Eric	NIST		Density Functional Theory Studies of Phase Transitions in Flexible Metal- organic Framework Materials
9	Fang, Hanjun	Georgia Institute of Technology	to be submitted at a later date	to be submitted at a later date
10	Gallington, Leighanne C	Argonne National Laboratory	Ana E. Platero-Prats, Karena W. Chapman	Structural effects of activation and catalysis on NU-1000 based catalysts
11	Gounder, Rajamani	Purdue University	Jason S. Bates, Michael J. Cordon, James W. Harris, Juan Carlos Vega-Vila	Kinetic studies of liquid-phase sugar isomerization reactions catalyzed by hydrophobic and hydrophilic Lewis acid zeolites
12	Huang, Wenyu	Iowa State University		Heterogeneous catalysis by metal nanocluster encapsulated in Metal- Organic Framework
13	lyoki, Kenta	Massachusetts Institute of Technology	Keiji Itabashi, Yoshihiro Kamimura, Masafumi Takase, Tatsuya Okubo	Seed-Directed, Heteroepitaxial Crystal Growth of Zeolites without Using Organic Structure-Directing Agents

14	Jelfs, Kim E	Imperial College London	M. Miklitz, V. Santolini, E. Berardo, K. E. Jelfs	Computational design of porous organic molecules for chemical separations
15	Kauer, Max	Ruhr University Bochum	Yuemin Wang	Vibrational Spectroscopic Studies on Defect-Engineered Metal-Organic Frameworks: Cu-HKUST-1 and Ru- HKUST-1
16	Khapli, Sachin	New York University Abu Dhabi	Sudhir Kumar Sharma, Ina Rianasari, Ramesh Jagannathan	Fabrication of Porous Ceramic Films with a Dual Hierarchy of Pores Through Supercritical CO2-assisted Nebulization
17	Kim, Wookdong	Center for Nanomaterials and Chemical Reactions, IBS	Yongbeom Seo, Youngjin Kim, Yonghyun Kwon, Seung Yoon Yang, and Ryong Ryoo	Aluminum Incorporation in Borosilicate and Pure-Silica MFI Zeolite Nanosponges: Their Brönsted Acidity and Catalytic Performance
18	Kim, Jaeheon	Center for Nanomaterials and Chemical Reactions	Joonsoo Chun, and Ryong Ryoo*	Ti-grafted MFI zeolite nanosheets as a highly efficient catalyst for epoxidation of bulky olefins using H2O2 as an oxidant
19	Kuila, Debasish	North Carolina A&T State University	V. Deshmane, R. Abrokwah, S. Owen	Effect of Mesoporous Silica and Titania Support on Catalytic Steam Reforming Reactions to Produce H2
20	Landskron, Kai	Lehigh University	Manik Mandal, Cong Liu, Fadi Haso, Yingwei Fei	Mesoporous boron nitride at high pressure
21	Lewis, Jennifer D	Massachusetts Institute of Technology	Jennifer D. Lewis, Stijn Van de Vyver, and Yuriy Román-Leshkov	C-C Coupling Catalyzed by Acid-Base Pairs in Lewis Acidic Zeolites
22	Liu, Junqiang	The Dow Chemical Company	Junqiang Liu, Edward Calverley, Chan Han	High throughput development of carbon molecular sieve for many industrial gas separations
23	Ma, Xiaowei	Dalhousie University	M. A. Rankin, L.M. Croll and J.R. Dahn	Nanoporous metal oxides as high capacity gas adsorbents
24	Martis, Vladimir	Surface Measurement Systems	Xiao Su, Lev Bromberg, Fritz Simeon, Ashfia Huq, Alan T. Hatton	Post-synthetic functionalization of Mg- MOF-74 using tetraethylene pentamine and its CO2/water vapor adsorption behavior
25	Miro Ramirez, Pere	Northwestern University	Peilin Liao, Melissa Barona and Randall Q. Snurr	Structure and Catalytic Activity of Well-Defined Metal Oxide Nanoclusters Grown in Nanoporous Materials
26	Morris, Russell E	University of St. Andrews	N/A	To be submitted at a later date
27	Nazarian, Dalar	Georgia Institute of Technology	Jeffrey Camp and David Sholl	Screening of Metal Organic Frameworks for Corrosive Odorant Removal from Natural Gas
28	Orazov, Marat	California Institute of Technology	Mark E. Davis	Zn Lewis sites in CIT-6 catalyze Diels- Alder reactions of ethylene and oxidized derivatives of 5- hydroxymethyl furfural (HMF)

29 Platero Prats, Ana Eva	Argonne National Laboratory, Advanced Photon Source	Ana E. Platero-Prats, Pete J. Chupas, Karena W. Chapman	Comprehensive in-situ studies of the zirconium node distortion in NU-1000
30 Rathi, Ashutosh	University of Massachusetts Amherst	John R. Edison, David M. Ford, Peter A. Monson	A Coarse-Grained Approach to Modeling Permporometry and Vapor Recovery with Mesoporous Membranes
31 Sekizkardes, Ali	U.S. Department of Energy National Energy and Technology Laboratory	Ali K. Sekizkardes, David Hopkinson	Porous Organic Polymers: Sorbent Materials for Post-Combustion Flue Gas Separation
32 Smaldone, Ronald A	University of Texas, Dallas	Christina M. Thompson, Sampath Alahakoon	Porous Organic Materials made from Polycyclic Aromatic Hydrocarbons
33 Tsung, Chia- Kuang	Boston College		Metal-organic framework controlled catalysis
34 Van Zee, Roger	National IInstitute of Standards & Technology	Laura Espinal, Matthias Thommes	NIST Facility for Adsorbent Characterization and Testing
35 Vattipalli, Vivek	Universtiy of Massachusetts Amherst	Xiaoduo Qi, Peter Monson, David Ford, Wei Fan	Experimental study on molecular transport in hierarchical porous materials
36 Vyas, Vijay S	Max Planck Institute for Solid State Research	Frederik Haase, Bettina V. Lotsch	Tuning Covalent Organic Frameworks for solar-fuel generation.
37 Yakovenko, Andrey A	Argonne National Laboratory	Gregory J. Halder	In Situ Powder Diffraction Studies of High-Pressure Gas Loading in Metal- Organic Frameworks
38 Zhao, Yanchuan	Massachusetts Institute of Technology	Yanchuan Zhao, Silvia Rocha and Timothy M. Swager	Mechanochemical synthesis of iptycene oligomers and dendrimers

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Chair: David Sholl Vice Chair: Guang Cao

> Important Note: The information in this Registration List is provided as a convenience to enable attendees to collaborate and keep in touch. In accordance with GRC policy, this information should not be shared with nonregistered attendees. Please respect the privacy of the other meeting attendees by not compiling email lists for the purpose of sending unsolicited emails, or by sharing their personal information without approval. Thank you.

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