

Mechanochemistry:
From Functional Solids
to Single Molecules
Faraday Discussion 170



21-23 May 2014
Montreal, Canada

Wednesday 21 May

11:00	Registration, Tea and Coffee	
12:00	Lunch	
12.45	Welcome and Introductions Tomislav Friščić	
12.55	Discussion Format Presentation Faraday Publishing Staff	
13.00	Introductory Lecture William Jones* <i>University of Cambridge, UK</i>	Paper 1
	Mechanochemistry of organic molecules, soft materials and pharmaceuticals Session Chair: Stuart James; Tomislav Friščić	
14:00	Liquid-assisted vortex grinding supports the single-step solid-state construction of a [2.2] paracyclophane Jelena Stojaković; Brian Farris; Leonard MacGillivray* <i>University of Iowa, USA</i>	Paper 15
14:05	Is the equilibrium composition of mechanochemical reactions predictable using computational chemistry? Peter Bygrave; David Case; Graeme Day* <i>University of Southampton, UK</i>	Paper 16
14:10	Two-step mechanochemical synthesis of porphyrins Hannah Shy; Paula Mackin; Andrea Orvieto; Deepa Gharbharan; Geneva Peterson; Nick Bampas; Tamara Hamilton* <i>Barry University, USA</i>	Paper 19
14:15	Discussion	
15.30	Afternoon tea	
16.00	Lightning Session	
16:30	Poster Session and Wine Reception	
18:30	Free Evening	

Thursday 22 May

	Mechanochemistry of inorganic compounds and coordination-based materials Session Chair: Elena Boldyreva; Leonard MacGillivray	
9:00	Mechanochemical synthesis of an organometallic compound: a high volume manufacturing method David Peters*; Richard Blair <i>ATMI, USA</i>	Paper 12
9:05	Mechanochemical preparation of copper iodide clusters of interest for luminescent devices Lucia Maini*; Paolo P. Mazzeo; Francesco Farinella; Valeria Fattori; Dario Braga <i>University of Bologna, Italy</i>	Paper 9
9:10	Mechanochemical synthesis and characterization of cocrystals and metal organic compounds Lisa Tröbs*; Franziska Emmerling <i>BAM Federal Institute for Materials Research and Testing, Germany</i>	Paper 10
9:15	Discussion	
10:30	Morning Tea	
11:00	The mechanically induced structural disorder in barium hexaferrite, BaFe₁₂O₁₉, and its impact on magnetism V. Šepélak*; M. Myndyk; R. Witte; J. Röder; D. Menzel; R. H. Schuster; H. Hahn; P. Heitjans; K.-D. Becker <i>Karlsruhe Institute of Technology, Germany</i>	Paper 11
11:05	Dry mechanochemical synthesis of alane from LiH and AlCl₃ Ihor Hlova; Shalabh Gupta; Jennifer Goldston; Takeshi Kobayashi; Marek Pruski; Vitalij Pecharsky* <i>The Ames Laboratory, USA</i>	Paper 13
11:10	Solvent-free mechanochemical synthesis of gold nanoparticles stabilized with amines or biomass matrix Monika Rak; Tomislav Friščić; Audrey Moores* <i>McGill University, Canada</i>	Paper 14
11:15	The dual role of sulfur-containing amino acid in the synthesis of IV–VI semiconductor nanocrystals: a mechanochemical approach Peter Baláž*; Matej Baláž; Mária Čaplovíčová; Anna Zorkovská; Lubomír Čaplovíč and Miroslav Psotka <i>Slovak Academy of Sciences, Slovakia</i>	Paper 8
11:20	Discussion	
13:00	Lunch	
	Mechanistic understanding, catalysis and scaling up of mechanochemistry Session Chair: Carsten Bolm; Peter Baláž	

14:00	Quantitative <i>in situ</i> and real-time monitoring of mechanochemical reactions Ivan Halasz*; Tomislav Friščić; Simon Kimber; Krunoslav Užarević; Andreas Puškarić; Cristina Mottillo; Patrick Julien; Vjekoslav Štrukil; Veijo Honkimäki; Robert Dinnebier <i>Rudjer Boskovic Institute, Croatia</i>	Paper 2
14:05	The scalability in the mechanochemical syntheses of edge functionalized graphene materials and biomass-derived chemicals Richard Blair*; Katerina Chagoya; Scott Biltek; Steven Jackson; Ashlyn Sinclair; Alexandra Taraboletti; David T. Restrepo <i>University of Central Florida, USA</i>	Paper 3
14:10	Application of twin screw extrusion to the manufacture of cocrystals: scale-up of AMG 517–sorbic acid cocrystal production Dominick Daurio; Karthik Nagapudi*; Lan Li; Peter Quan; Fernando Alvarez-Núñez <i>Amgen Inc, USA</i>	Paper 4
14:15	Discussion	
15:30	Afternoon Tea	
16.00	Self-sustaining reactions as a tool to study mechanochemical activation Laszlo Takacs <i>University of Maryland, USA</i>	Paper 5
16:05	Scale-up of organic reactions in ball mills: process intensification with regard to energy efficiency and economy of scale Achim Stolle*; Robert Schmidt; Katharina Jacob <i>Friedrich-Schiller University Jena, Germany</i>	Paper 6
For discussion via the forum	Advances in elucidating mechanochemical complexities via implementation of a simple organic system Adam Michalchuk*; Ivan Tumanov; Valeri Drebuschak; Elena Boldyreva <i>Novosibirsk State University, Russia; University of Edinburgh, UK; Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia</i>	Paper 7
16:10	Discussion	
17.00	Close of sessions	
19:00	Pre-dinner Drinks	
19:30	Conference Dinner	

Friday 23 May

Sonication and macromolecular mechanochemistry Session Chair: James Mack; Richard Blair		
09:00	Enhancing covalent mechanochemistry in bulk polymers using electrospun ABA triblock copolymers A. L. Black Ramirez; A. K. Schmitt; M. K. Mahanthappa; S. L. Craig* <i>Duke University, USA</i>	Paper 20
09:05	Mechanically induced silyl ester cleavage under acidic conditions investigated by AFM-based single-molecule force spectroscopy in the force-ramp mode Sebastian Schmidt; Michael Pill; Alfred Kersch; Hauke Clausen-Schaumann; Martin Beyer* <i>Christian-Albrechts-Universität zu Kiel, Germany</i>	Paper 22
For discussion via the forum	Increasing the energy yield of mechanochemical transformations: selected case studies Anatoly Politov*; Olga Golyazimova <i>Novosibirsk State University, Russia; Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia</i>	Paper 21
09:10	Discussion	
10:00	Morning Tea	
10:30	Triboelectricity in insulators: evidence for a mechanochemical mechanism Lia Beraldo da Silveira Balestrin; Douglas Del Duque; Douglas Soares da Silva; Fernando Galembeck* <i>Brazilian National Nanotechnology Laboratory, Brazil</i>	Paper 24
10:35	Mechanochemical production of phenyl cations through heterolytic bond scission Tomohiro Shiraki; Charles Diesendruck; Jeffrey Moore <i>University of Illinois at Urbana-Champaign</i>	Paper 25
10:40	Discussion	
11:30	Concluding remarks Kenneth Suslick* <i>University of Illinois at Urbana-Champaign</i>	Paper 26
12:15	Acknowledgements	
12:45	Close of meeting and lunch	