

**ICMR Workshop on  
Design and Synthesis of New Materials**

Santa Barbara, August 1 – 2, 2008

**Friday, August 1<sup>st</sup>**

8:20 – 8:30	<b>Welcoming remarks</b>
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*Mike Treacy and Igor Rivin*

**Structure enumeration methods**

8:30 – 9:00	<b>Tangling nets with knots and ravel</b>
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*Stephen Hyde*

Department of Mathematics, The Australian National University, Canberra  
ACT 0200, Australia

9:00 – 9:10	<b>Discussion</b>
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9:10 – 9:40	<b>A mix-and-match approach to the discovery of new potential framework types</b>
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*Olaf Delgado Friedrichs*

Research & Visualization, Vizlab, ANU Supercomputer Facility  
Australian National University, Canberra, Australia

9:40 – 9:50	<b>Discussion</b>
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9:50 – 10:20    **Break**

10:20 – 10:50	<b>The next generation of computational and mathematical tools – a bird's eye view</b>
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*Igor Rivin*

Mathematics Department, Temple University, Philadelphia, PA 19122

10:50 – 11:00	<b>Discussion</b>
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11:00 – 11:30	<b>The Monte Carlo sampling approach to construction of a database of hypothetical zeolite frameworks</b>
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*Michael W. Deem*

Rice University, Houston, TX 77005 USA

11:30 – 11:40	<b>Discussion</b>
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11:40 – 12:10	<b>Surfaces, tilings, nets and circle packings in the EPINET project</b>
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*Stuart Ramsden*

Research & Visualization, Vizlab, ANU Supercomputer Facility  
Australian National University, Canberra, Australia

12:10 – 12:20	<b>Discussion</b>
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12:30 – 1:30     **Lunch**

1:30 – 2:00     **Designer zeolites**

*Mike Treacy*

Department of Physics, Arizona State University, Tempe AZ 85287

2:00 – 2:10     **Discussion**

2:10 – 2:40     **Hypothetical zeolites – analysis of structures**

*Martin Foster*

Stark Investments 1000 N. Water Street, Milwaukee, WI 53202

2:40 – 2:50     **Discussion**

2:50 – 3:20     **Towards the designed synthesis of zeolitic nanoporous materials**

*Jihong Yu*

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry  
College of Chemistry, Jilin University, Changchun 130012, P. R. China

3:20 – 3:30     **Discussion**

3:30 – 4:00     **Break**

## Synthesis strategies

4:00 – 4:30     **High throughput synthesis of zeolites**

*Karl Strohmaier*

ExxonMobil Research & Engineering Company  
1545 Route 22 East, Annandale, NJ 08801

4:30 – 4:40     **Discussion**

4:40 – 5:10     **Combinatorial zeolite synthesis using the charge density mismatch approach**

*Bob Broach*

UOP LLC, 25 E. Algonquin Rd, Des Plaines, IL, USA 60017

5:10 – 5:20     **Discussion**

6:00             **Workshop Dinner**

**Saturday, August 2nd**

**Synthesis strategies (cont.)**

8:30 – 9:00	<b>TBA</b> <i>Omar Yaghi</i> Department of Chemistry & Biochemistry UCLA Los Angeles, CA 90095-1569
9:00 – 9:10	<b>Discussion</b>

9:10 – 9:40	<b>Using confinement and interfaces in the synthesis and use of nanophase structures</b> <i>Galen D. Stucky</i> Department of Chemistry and Biochemistry, Materials Department University of California, Santa Barbara, California
9:40 – 9:50	<b>Discussion</b>

9:50 – 10:20 **Break**

10:20 – 10:50	<b>Novel open-framework germanates built from inorganic clusters</b> <i>Xiaodong Zou and Charlotte Bonneau,</i> Structural Chemistry and Berzelii Centre EXSELENT on Porous Materials Stockholm University, SE-106 91 Stockholm, Sweden
10:50 – 11:00	<b>Discussion</b>

**Framework and structure analysis**

11:00 – 11:30	<b>Recent findings in the search of polycatenated and interpenetrated materials</b> <i>Davide M. Proserpio</i> Dipartimento di Chimica Strutturale e Stereochimica Inorganica Universita' di Milano, Via Venezian, 21 - 20133 Milano, Italy
11:30 – 11:40	<b>Discussion</b>

11:40 – 12:10	<b>Computer analysis of periodic nets: methods, software and databases</b> <i>Vladislav A. Blatov</i> Samara State University, Ac. Pavlov St. 1, Samara 443011, Russia
12:10 – 12:20	<b>Discussion</b>

12:30 – 1:30 **Lunch**

1:30 – 2:00	<b>Flexibility and rigidity in network structures</b> <i>Mike Thorpe</i> Department of Physics, Arizona State University, Tempe AZ 85287
2:00 – 2:10	<b>Discussion</b>

2:10 – 2:40	<b>Molecular simulations of shape selectivity in zeolites</b> <i>Berend Smit</i> Department of Chemical Engineering and Department of Chemistry University of California, Berkeley CA 94720-1462
2:40 – 2:50	<b>Discussion</b>

2:50 – 3:20     **Break**

3:20 – 3:50	<b>A taxonomy of nets and crystal design</b> <i>Mike O’Keeffe</i> Department of Chemistry, Arizona State University, Tempe AZ 85287
3:50 – 4:00	<b>Discussion</b>

4:00 – 4:30	<b>TBA</b> <i>Richard Catlow</i> Department of Chemistry, University College London 20 Gordon Street, London WC1H 0AJ, United Kingdom
4:30 – 4:40	<b>Discussion</b>

4:40 – 5:00     **Wrap-up discussion**

**Free evening**