

## Ahmed E. Ismail

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### CONTACT

INFORMATION AICES Graduate School  
RWTH Aachen University  
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### EDUCATION

#### **Massachusetts Institute of Technology**

Ph.D. in Chemical Engineering, conferred June 2005

- Thesis: *Multiresolution methods for materials modeling via coarse-graining*
- Advisors: Gregory C. Rutledge and George Stephanopoulos

#### **Yale University**

B.S. *magna cum laude* in Chemical Engineering with Distinction, 1998

### PROFESSIONAL AND RESEARCH EXPERIENCE

#### **Junior Professor**

*RWTH Aachen University, Aachen, NW, Germany*

Faculty of Mechanical Engineering, 2010–present

- Appointment in Aachen Verfahrenstechnik
- Junior Professor in Tailor-Made Fuels from Biomass Cluster of Excellence
- Associated Young Researcher in AICES Graduate School

#### **Senior Member of Technical Staff**

*Sandia National Laboratories, Carlsbad, NM*

Performance Assessment Department, 2006–2010

- Molecular dynamics simulations of functionalized silica nanoparticles
- Molecular dynamics simulations of PDMS-water interface
- Transport modeling, geochemical modeling, and performance assessment for the Waste Isolation Pilot Plant

#### **Postdoctoral Appointee**

*Sandia National Laboratories, Albuquerque, NM*

Computational Materials Science and Engineering Department, 2005–2006

Advisors: Gary Grest and Mark Stevens

- Molecular dynamics simulations of water liquid-vapor interface
- Molecular dynamics simulations of dipolar systems

### OTHER RESEARCH EXPERIENCE

#### **Computational Sciences Graduate Fellowship Practicum**

*Oak Ridge National Laboratory, Oak Ridge, TN*

Computational Chemical Sciences, Computer Science and Math Division, 2002

Supervisor: Bill Shelton

#### **Undergraduate Research Assistant**

*Yale University, New Haven, CT*

Complex Fluids Laboratory, Department of Chemical Engineering, 1997-1998

Supervisor: Michael Loewenberg

### **Undergraduate Research Scholar**

*National Institutes of Health, Bethesda, MD*

Analytical Chemistry Laboratory, National Institute of Mental Health, 1997

Supervisors: P. F. Morrison and M. P. Heyes

### TEACHING EXPERIENCE

#### **RWTH Aachen University**

- Lecturer, Winter Semester 2010/11 Co-lecturer for Simulationstechnik II, required course for second-year undergraduates in Computational Engineering Science.
- Lecturer, Spring Semester 2011 Lecturer for Introduction to Molecular Simulation, a technical elective for master's students in Mechanical Engineering

#### **Massachusetts Institute of Technology**

- Instructor-G, Fall 2004  
10.10, *Introduction to Chemical Engineering*, a required undergraduate course.
- Graduate Teaching Assistant, Fall 2001  
Teaching Assistant for 10.40, *Chemical Engineering Thermodynamics*, a required course for first-year graduate students.

#### **Yale University**

- Facilitator, STARS Program 1997–1998  
Teaching assistant for Math 112 and 115, *Calculus of Functions of a Single Variable I and II* and Math 120, *Calculus of Functions of Several Variables*.

### PUBLICATIONS

#### Refereed Publications:

1. **AE Ismail**, F Pierce, and GS Grest. DIFFUSION OF SMALL PENETRANTS IN POLYBUTADIENES. Published online in *Mol. Phys.* DOI: 10.1080/00268976.2011.608085 (2011).
2. MB Nemer, Y-L Xiong, **AE Ismail**, J-H Jang, S Johnsen, and T MacDonald. SOLUBILITY OF  $\text{Fe}_2(\text{OH})_3\text{Cl}$  (PURE-IRON END-MEMBER OF HIBBINGITE) IN 0.1–5 M NaCl. *Chem. Geol.* **280**, 26 (2010).
3. **AE Ismail**, JA Greathouse, PS Crozier, and SM Foiles. THE EFFECT OF ELECTRON-ION COUPLING ON SIMULATIONS OF RADIATION DAMAGE IN A PYROCHLORE WASTEFORM. *J. Phys.: Cond. Matt.* **22**, 225405 (2010).
4. JMD Lane, **AE Ismail**, ME Chandross, CD Lorenz, and GS Grest. FORCES BETWEEN FUNCTIONALIZED SILICA NANOPARTICLES IN SOLUTION. *Phys. Rev. E*, **79**, 050501R (2009).

5. **AE Ismail**, GS Grest, DR Heine, MJ Stevens, and M Tsigie. INTERFACIAL STRUCTURE AND DYNAMICS OF SILOXANE SYSTEMS: PDMS–VAPOR AND PDMS–WATER. *Macromolecules*, **42**, 3186 (2009).
6. **AE Ismail**, M Tsigie, PJ in 't Veld and GS Grest. SURFACE TENSION OF NORMAL AND BRANCHED ALKANES. *Mol. Phys.*, **105**, 3155 (2007).
7. PJ in 't Veld, **AE Ismail**, and GS Grest. APPLICATION OF EWALD SUMMATIONS TO LONG-RANGE DISPERSION FORCES. *J. Chem. Phys.*, **127**, 144711 (2007).
8. **AE Ismail**, GS Grest, and MJ Stevens. STRUCTURE AND DYNAMICS OF WATER NEAR THE INTERFACE WITH OLIGO(ETHYLENE OXIDE) SELF-ASSEMBLED MONOLAYERS. *Langmuir*, **23**, 8508 (2007).
9. **AE Ismail**, GS Grest, and MJ Stevens. CAPILLARY WAVES AT THE LIQUID-VAPOR INTERFACE AND THE SURFACE TENSION OF WATER. *J. Chem. Phys.*, **125**, 014702 (2006).
10. **AE Ismail**, GC Rutledge, and G Stephanopoulos. TOPOLOGICAL COARSE-GRAINING OF POLYMER CHAINS USING WAVELET-ACCELERATED MONTE CARLO. I. FREELY-JOINTED CHAINS. *J. Chem. Phys.*, **122**, 234901 (2005).
11. **AE Ismail**, G Stephanopoulos, and GC Rutledge. TOPOLOGICAL COARSE-GRAINING OF POLYMER CHAINS USING WAVELET-ACCELERATED MONTE CARLO. II. SELF-AVOIDING CHAINS. *J. Chem. Phys.*, **122**, 234902 (2005).
12. **AE Ismail**, G Stephanopoulos, and GC Rutledge. WAVELET-ACCELERATED MONTE CARLO SAMPLING OF POLYMER CHAINS. *J. Polym. Sci. B: Polym. Phys.*, **43**, 897 (2005). (Invited)
13. **AE Ismail**, GC Rutledge, and G Stephanopoulos. USING WAVELET TRANSFORMS FOR MULTIREOLUTION MATERIALS MODELING. *Comp. Chem. Eng.*, **29**, 689 (2005). (Invited)
14. **AE Ismail** and M Loewenberg. LONG-TIME EVOLUTION OF A DROP SIZE DISTRIBUTION BY COALESCENCE IN A LINEAR FLOW. *Phys. Rev. E.*, **69**, 046307 (2004).
15. **AE Ismail**, GC Rutledge, and G Stephanopoulos. MULTIREOLUTION ANALYSIS IN STATISTICAL MECHANICS. I. USING WAVELETS TO CALCULATE THERMODYNAMIC PROPERTIES. *J. Chem. Phys.*, **118**, 4414 (2003).
16. **AE Ismail**, G Stephanopoulos, and GC Rutledge. MULTIREOLUTION ANALYSIS IN STATISTICAL MECHANICS. II. THE WAVELET TRANSFORM AS A BASIS FOR MONTE CARLO SIMULATIONS ON LATTICES. *J. Chem. Phys.*, **118**, 4424 (2003).

Conference Proceedings:

1. Y Xiong, J Nowak, LH Brush, **AE Ismail**, and JL Long. ESTABLISHMENT OF UNCERTAINTY RANGES AND PROBABILITY DISTRIBUTIONS OF ACTINIDE SOLUBILITIES FOR PERFORMANCE ASSESSMENT IN THE WASTE

ISOLATION PILOT PLANT *Materials Research Society Symposium Proceedings, Vol. 1265: Scientific Basis for Nuclear Waste Management XXXIV*. San Francisco, CA, 5-9 April 2010. In press.

2. DJ Clayton and **AE Ismail**. IMPACT OF PROPOSED DISTURBED ROCK ZONE CONCEPTUAL MODEL MODIFICATIONS TO THE 2007 WASTE ISOLATION PILOT PLANT PERFORMANCE ASSESSMENT ON LONG-TERM REPOSITORY PERFORMANCE. *Proceedings of the 2008 Waste Management Symposium*. Phoenix, AZ, 25-28 February 2008.

PRESENTATIONS    Invited Talks:

1. **AE Ismail**, ATOMISTIC SIMULATIONS OF STRUCTURE AND DYNAMICS OF POLYMERS AT INTERFACES. Institute für Geometrie und Praktische Mathematik, RWTH Aachen University, Aachen, Germany. 27 October 2011.

APPLYING COMPUTATIONAL MATERIALS SCIENCE TO BIOFUELS PRODUCTION. Argonne National Laboratory, Argonne, IL. 14 October 2011.

LESSONS LEARNED FROM LARGE-SCALE SIMULATIONS AT “INTERFACES”. Trends in Computational Science and Engineering: Foundations of Modeling and Simulation. ASIM Workshop 2011. TU Mnchen, Garching, Germany, 14–16 March 2011.

2. **AE Ismail** DIFFUSION OF SMALL PENETRANTS IN POLYMERS. Max-Planck Institut für Polymerforschung, Mainz, Germany. 25 January 2011.

3. **AE Ismail**, G Stephanopoulos, and GC Rutledge, COARSE-GRAINED MODELING OF POLYMERS USING WAVELET ACCELERATED MONTE CARLO SIMULATION. American Chemical Society, 230th National Meeting, Washington, DC, 28 August–1 September 2005.

4. **AE Ismail**, GC Rutledge, and G Stephanopoulos. A NEW WAVELET-BASED PARADIGM FOR HIERARCHICAL COARSE-GRAINING APPLIED TO MATERIALS MODELING. American Control Conference, Boston, MA, 30 June–2 July 2004.

5. **AE Ismail**, G Stephanopoulos, and GC Rutledge. HIERARCHICAL MODELING OF POLYMER MODELS. NIH Undergraduate Scholarship Program Research Festival. Bethesda, MD, 7 August 2003.

6. **AE Ismail**, G Stephanopoulos, and GC Rutledge. WAVELET-ACCELERATED MONTE CARLO SIMULATIONS OF COARSE-GRAINED LATTICE POLYMER MODELS. Department of Energy Computational Science Graduate Fellowship Conference, Washington D. C., 15–17 July 2003.

Contributed Talks:

1. **AE Ismail**. MOLECULAR SIMULATION OF THE FORMATION AND STRUCTURE OF NaCl NANOPARTICLES. MRS Spring Meeting, San Francisco, CA, 5-9 April 2010.

2. **AE Ismail**, F Pierce, MC Celina, and GS Grest. DIFFUSION OF SMALL PENETRANTS THROUGH POLYBUTADIENES. APS March Meeting, Portland, OR, 15-19 March 2010.
3. **AE Ismail**, GS Grest, DR Heine, MJ Stevens, and M Tsigie. DIFFUSION OF WATER THROUGH METHYL- AND HYDROXYL-TERMINATED POLY(DIMETHYLSILOXANE). APS March Meeting, Pittsburgh, PA, 16-20 March 2009.
4. JMD Lane, **AE Ismail**, ME Chandross, and GS Grest. ATOMISTIC SIMULATIONS OF HYDRODYNAMIC AND INTERACTION FORCES ON FUNCTIONALIZED SILICA NANOPARTICLES. APS March Meeting, Pittsburgh, PA, 16-20 March 2009.
5. JMD Lane, **AE Ismail**, ME Chandross, and GS Grest. FORCES BETWEEN FUNCTIONALIZED SILICA NANOPARTICLES. AIChE Annual Meeting, Philadelphia, PA, 16-20 November 2008.
6. **AE Ismail** and DJ Clayton. IMPACT OF PROPOSED DISTURBED ROCK ZONE CONCEPTUAL MODEL MODIFICATIONS TO THE 2007 WASTE ISOLATION PILOT PLANT PERFORMANCE ASSESSMENT ON LONG-TERM REPOSITORY PERFORMANCE. 2008 Waste Management Symposium, Phoenix, AZ, 25-28 February 2008.
7. **AE Ismail**, GS Grest, DR Heine, MJ Stevens, and M Tsigie. INTERFACIAL PROPERTIES OF PDMS-WATER SYSTEMS. AIChE Annual Meeting, Salt Lake City, UT, 4-9 November 2007.
8. PJ in 't Veld, **AE Ismail**, and GS Grest. APPLICATION OF EWALD SUMMATIONS TO LONG-RANGE DISPERSION FORCES. ACS National Meeting, Boston, CT, 19-23 August 2007.
9. **AE Ismail**, GS Grest, and MJ Stevens. STRUCTURE AND DYNAMICS OF WATER NEAR THE INTERFACE WITH OLIGO(ETHYLENE OXIDE) SELF-ASSEMBLED MONOLAYERS. APS March Meeting, Denver, CO, 5-9 March 2007. ACS National Meeting, Boston, CT, 19-23 August 2007.
10. **AE Ismail**, GS Grest, and MJ Stevens. CAPILLARY WAVES AT THE LIQUID-VAPOR INTERFACE AND THE SURFACE TENSION OF WATER. AIChE Annual Meeting, San Francisco, CA, 13-17 November 2006.
11. MJ Stevens, GS Grest, M Chandross, **AE Ismail**, and CD Lorenz. SIMULATIONS OF WATER AT THE INTERFACE WITH SELF-ASSEMBLED MONOLAYERS. ACS National Meeting, San Francisco, CA, 10-14 September 2006.
12. **AE Ismail**, G Stephanopoulos, and GC Rutledge. CHARACTERISTICS OF PARAMETER REDUCTION IN COARSE-GRAINED MODELS OF POLYMER CHAINS. AIChE Annual Meeting, Austin, TX, 8-12 November 2004.
13. **AE Ismail**, G Stephanopoulos, and GC Rutledge. COARSE-GRAINING OF POLYMER MODELS USING WAVELET-ACCELERATED MONTE CARLO. APS March Meeting, Montréal, PQ, Canada, 22-26 March 2004.

14. **AE Ismail**, GC Rutledge, and G Stephanopoulos. MULTIREOLUTION ANALYSIS USING WAVELETS TO CALCULATE THERMODYNAMIC PROPERTIES. AIChE Annual Meeting, Indianapolis, IN, 3–8 November 2002.
15. **AE Ismail**. MULTIREOLUTION METHODS FOR MATERIALS MODELING. Departmental Seminar, MIT Department of Chemical Engineering, Cambridge, MA, 19 March 2001.

Poster Presentations

1. **AE Ismail**, LH Brush, J-H Jang, SR Johnsen, MB Nemer, and Y-L Xiong. DETERMINATION OF UNCERTAINTIES FOR +III AND +IV ACTINIDE SOLUBILITIES IN THE WIPP GEOCHEMISTRY MODEL FOR THE 2009 COMPLIANCE RECERTIFICATION APPLICATION American Geophysical Union Fall Meeting, San Francisco, CA, 14-18 December 2009.
2. **AE Ismail**, LH Brush, J-H Jang, SR Johnsen, MB Nemer, and Y-L Xiong. DETERMINATION OF PITZER PARAMETERS FOR Pb(II) AND Fe(II) SOLUBILITIES IN CONCENTRATED BRINES IN THE PRESENCE OF ENVIRONMENTAL LIGANDS AIChE Annual Meeting, Nashville, TN, 9-13 November 2009.
3. P.J. in 't Veld, **AE Ismail**, and GS Grest. APPLICATION OF EWALD SUMMATIONS TO LONG-RANGE DISPERSION FORCES. AIChE Annual Meeting, Salt Lake City, UT, 12-16 November 2007.
4. **AE Ismail**, GS Grest, and MJ Stevens. STRUCTURE AND DYNAMICS OF WATER AT THE INTERFACE WITH POLY(ETHYLENE GLYCOL) SELF-ASSEMBLED MONOLAYERS. Gordon Research Conference on Polymer Physics. New London, CT, 23–28 July 2006.
5. **AE Ismail**, G Stephanopoulos, and GC Rutledge. MULTIREOLUTION MODELING OF POLYMERS USING WAVELET-ACCELERATED MONTE CARLO. ACS WORKSHOP ON MOLECULAR MODELING OF MACROMOLECULES, Hilton Head, SC, 17-20 March 2004.
6. **AE Ismail**, GC Rutledge, and G Stephanopoulos. MULTIREOLUTION ANALYSIS IN STATISTICAL MECHANICS USING THE WAVELET-ACCELERATED MONTE CARLO ALGORITHM. Forum on Molecular Modeling and Simulation, Keystone, CO, 6-11 July 2003.
7. **AE Ismail** and M Loewenberg. GROWTH OF DROP-SIZE DISTRIBUTION BY COALESCENCE IN LINEAR FLOWS. AIChE National Meeting, Miami, FL, 19 November 1998.
8. **AE Ismail**, PF Morrison, and MP Heyes. ASSESSING THE VALIDITY OF MICRODIALYSIS TO PREDICT CONCENTRATION PROFILES OF INHIBITION REACTIONS. National Institutes of Health Poster Day, August 1997.

SUPERVISION

Postdoctoral Associates

- Brooks D. Rabideau (July 2010–Present): Transport properties of ionic liquid–cellulose mixtures

Doctoral Students

- Amir Abolhoseini Niazi (July 2010–Present): Thermodynamic properties of ionic liquid–water systems

Master’s Students

- Rolf Isele-Holder (March–July 2011): Establishing a link between COSMO-RS and Molecular Dynamics Simulations

HONORS AND AWARDS

Department of Energy Computational Science Graduate Fellow (2000-2004).

Department of Defense (NDSEG) Fellow (1998-2000).

Offered NSF, Ford Foundation, and GEM Fellowships for graduate study (1998).

Henry Prentiss Becton Prize for Excellence in Engineering and Applied Science (1998).

American Society of Military Engineers Scholarship (1997-1998).

Chemical Engineering Junior Prize (1997).

National Institutes of Health Undergraduate Scholarship (1996-1997).

American Chemical Society Scholarship (1995-1998).

Benjamin Barge Prize in Mathematics (1995, 1996).

Member of Sigma Xi (1999) and Tau Beta Pi, Connecticut Alpha Chapter (1996)

PROFESSIONAL SOCIETIES AND ACTIVITIES

Professional Memberships

- American Chemical Society
- American Institute of Chemical Engineers
- American Physical Society
- Materials Research Society
- Society for Industrial and Applied Mathematics

Other Activities

- Referee for *Fluid Phase Equilibria*, *Journal of Chemical Physics*, *Journal of Polymer Science Part B: Polymer Physics*, *Langmuir*, *Macromolecules*, and *Polymer*
- Organizing Committee, First Aachen Conference on Computational Engineering Science (AC.CES 2011)
- Polymers Area Vice Chair and Chair-Elect, American Institute of Chemical Engineers, 2011-2012
- Session Chair and Co-Chair, American Institute of Chemical Engineers, 2003, 2008-2010

*Last updated February 4, 2013.*