

ATEEQUE MALANI

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Department of Chemical Engineering
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Professional Experience

- 07/2012 - Present **Assistant Professor**, Indian Institute of Technology (IIT) Bombay, Mumbai, India.
09/2010 - 06/2012 **Postdoctoral Associate**, Massachusetts Institute of Technology (MIT), Cambridge, USA.
03/2009 - 08/2010 **Postdoctoral Research Associate**, University of Massachusetts (UMASS), Amherst, USA.

Education

- 2004-2009 **Ph.D. (Chemical Engineering)**, Indian Institute of Science (IISc), Bangalore, India.
Thesis : Structure and dynamics of interfacial and confined water
Advisor : Prof. K. Ganapathy Ayappa
- 2002-2004 **M. Tech. (Chemical Engineering)**, Indian Institute of Technology (IIT), Bombay, India.
CGPA : 9.3/10 (Rank: 3rd in class)
Thesis : Liquid flow in cylindrical microchannels.
Advisors : Kartic. C. Khilar and Mahesh Triumkudulu
- 1998-2002 **B.E. (Chemical Engineering)**, S G B Amravati University, India.
Score : 76.2% (Rank: 1st in University)

Awards and Honours

- 2014 Best Alumni Award, JD Inst. of Engg. & Tech., Yavatmal, India.
- 2012 IIT Bombay Young Faculty Award.
- 2006 Indo-US student exchange fellowship to conduct research at University of Illinois at Chicago (UIC) for a duration of six months.
- 2007 Travel grant from Council for Scientific and Industrial Research (CSIR), India to attend international conference.
- 2007 Travel grant from Department of Science and Technology (DST), India to attend international conference.
- 2007 Travel grant from Indian National Science Academy (INSA), India to attend international conference.
- 2004-2009 Senior Research Fellowship from Ministry of Human Resource and Development (MHRD), India.
- 2002-2004 Junior Research Fellowship from MHRD, India.

Teaching Experience

May 2018	Instructor, Introduction to Numerical Analysis, Chemical Engg., IIT Bombay.
Aug 2017	Instructor, Advanced Thermodynamics, Chemical Engg., IIT Bombay.
Jan 2017	Instructor, Colloids & Interfacial Engineering, Chemical Engg., IIT Bombay.
Aug 2016	Instructor, Advanced Thermodynamics, Chemical Engg., IIT Bombay.
Jan 2016	Instructor, Multiscale Simulations, Chemical Engg., IIT Bombay.
Aug 2015	Instructor, Introduction to Numerical Analysis, Chemical Engg., IIT Bombay.
Jan 2015	Instructor, Multiscale Simulations, Chemical Engg., IIT Bombay.
Aug 2014	Instructor, Introduction to Numerical Analysis, Chemical Engg., IIT Bombay.
Jan 2014	Instructor, Multiscale Simulations, Chemical Engg., IIT Bombay.
Aug 2013	Instructor, Introduction to Numerical Analysis, Chemical Engg., IIT Bombay.
Jan 2013	Instructor, Introduction to Numerical Analysis, Chemical Engg., IIT Bombay.
Aug 2012	Instructor, Chemical Engineering Laboratory, Chemical Engg., IIT Bombay.
2008	Guest Instructor, Statistical Thermodynamics, Chemical Engg., IISc Bangalore
2002-2009	Teaching Assistant at IIT Bombay and IISc Bangalore.

Professional Activities

- Conference Organizer, Mumbai-Pune Soft Matter meeting, March 2016 IIT Bombay, India.
- Session Chair, Modeling of Interfacial Systems, 2016 AIChE Annual Meeting, San Francisco, USA.
- Session Chair, Solid-Liquid Interfacial System, 2016 AIChE Annual Meeting, San Francisco, USA.
- Session Chair, Wetting and Adhesion, CompFlu-2016, Pune, India..
- Session Chair, Modeling of Interfacial Systems, 2014 AIChE Annual Meeting, Atlanta, USA.
- Session Co-chair, Anisotropic Particles I, 2014 AIChE Annual Meeting, Atlanta, USA.
- Session Co-chair, Multiscale and Coarse-Grained Modeling of Polymers, 2014 AIChE Annual Meeting, Atlanta, USA.
- Session Chair, Modeling and Simulations of Polymer I, 2013 AIChE Annual Meeting, San Francisco, USA.
- Session Chair, Molecular Simulation and Modeling of Complex Molecules II, 2012 AIChE Annual Meeting, Pittsburgh, USA.
- Session Co-chair, Molecular Simulation and Modeling of Complex Molecules I, 2012 AIChE Annual Meeting, Pittsburgh, USA.
- Member, American Physics Society (APS), USA. (2012 onwards)
- Member, American Institute of Chemical Engineers (AIChE), USA. (2009 onwards)
- Reviewer for Langmuir, Scientific Reports, Computational Material Science and other Journals.

Community Outreach

April 2018 Career guidance seminar to 10th and 12th grade students at Kalyan, Mumbai.

April 2018 Career guidance seminar to 10th and 12th grade students at Mumbra, Mumbai.

Dec. 2017 Career guidance seminar to 10th and 12th grade students at Yavatmal.

Publications

19. S Adapa, D R Swamy, S Kancharla, S Pradhan and **A Malani**, Role of mono- and divalent surface cations on structure and adsorption behavior of water on mica surface, **under review**.
18. S Adapa and **A Malani**, Role of hydration energy and co-ions association on monovalent and divalent cations adsorption at mica-aqueous interface, *Scientific Reports*, **2018**, **Accepted**.
17. M Singh, N Rampal and **A Malani**, Structural behaviour of isolated asphaltene molecules at the oil-water interface, *Energy & Fuels*, **2018**, **Accepted**.
16. A Sharma, R Babarao, N V Medhekar and **A Malani**, Methane adsorption and separation in slipped and functionalized covalent organic frameworks, *Ind. Engg. Chem. Res.*, **2018**, *57*, 4767.
15. I Shere and **A Malani** Polymerization kinetics of a multi-functional silica precursor studied using a novel Monte Carlo simulation technique, *Phys. Chem. Chem. Phys.*, **2018**, *20*, 3554.
14. D Kaleeswaran, R Antony, A Sharma, **A Malani** and R Murugavel Catalysis and CO₂ capture by palladium incorporated covalent organic frameworks, *Chem. Plus. Chem.*, **2017**, *82*, 1253.
13. A Sharma, **A Malani**, N V Medhekar and R Babarao, CO₂ adsorption and separation in covalent organic frameworks with interlayer slipping, *Cryst. Eng. Comm.*, **2017**, *19*, 6950.
12. A Sharma, R Huang, **A Malani** and R Babarao, Computational materials chemistry for carbon capture using porous materials, *J. Phys. D*, **2017**, *50*, 463002.
11. R Debbarma and **A Malani**, Comparative study of water adsorption on a H⁺ and K⁺ ion exposed mica surface: Monte Carlo simulation study, *Langmuir*, **2016**, *32*, 1034.
10. **A Malani**, A Raghavanpillai, E B Wysong and G C Rutledge, Can dynamic contact angle be measured using molecular modeling?, *Phys. Rev. Lett.*, **2012**, *109*, 184501.
9. **A Malani** and K G Ayappa, Confined fluids in a Janus pore: Influence of surface asymmetry on structure and solvation forces, *Mol. Sim.*, **2012**, *38*, 1114.
8. **A Malani** and K G Ayappa, Molecular jump mechanism of water near mica surface, *J. Chem. Phys.*, **2012**, *136*, 194701.
7. **A Malani**, S M Auerbach and P A Monson, Monte Carlo simulations of silica polymerization and network formation, *J. Phys. Chem. C*, **2011**, *115*, 15988.
6. **A Malani**, S M Auerbach and P A Monson, Probing the mechanism of silica polymerization at ambient temperatures using Monte Carlo simulations, *J. Phys. Chem. Lett.*, **2010**, *1*, 3219.
5. **A Malani**, S Murad and K G Ayappa, Hydration of ions under confinement, *Mol. Sim.*, **2010**, *36*, 579.
4. **A Malani**, K G Ayappa and S Murad, Influence of hydrophilic surface specificity on the structural properties of confined water, *J. Phys. Chem. B*, **2009**, *113*, 13825.
3. **A Malani** and K G Ayappa, Adsorption isotherms of water on mica: Redistribution and film growth, *J. Phys. Chem. B*, **2009**, *113*, 1058.

2. K G Ayappa, **A Malani**, K Patil and F Thakkar, Molecular simulations: Probing systems from the nanoscale to mesoscale, *J. Indian I. Sci.*, **2007**, 87, 35.
1. **A Malani**, K G Ayappa and S Murad, Effect of confinement on the hydration and solubility of NaCl in water, *Chem. Phys. Lett.*, **2006**, 431, 88.

Oral Presentations

- 2018 2nd ISFE, Hiroshima University, Japan (**Invited**)
- Nanoporous materials for adsorbed natural gas (A Sharma, R Babarao, N Medhekar and **A Malani**)
- 2018 BASF, Ludwigschafen, Germany (**Invited**)
- Multiscale modelling of self assembly and interfacial phenomena (**A Malani**)
- 2018 10th LIBLICE, Prague, Czech Republic
- Adsorption of ions at solid-liquid interfaces (S Adapa and **A Malani**)
- 2018 30th ESAT, Prague, Czech Republic
- Multiscale modelling of CO₂ and CH₄ separation and storage in 2D-COF materials (A Sharma, R Babarao, N Medhekar and **A Malani**)
- 2018 BASF Innovation Campus, Mumbai, India (**Invited**)
- Multiscale modelling of self assembly and interfacial phenomena (**A Malani**)
- 2017 CCP5 - Annual General Meeting, University of Strathclyde, UK.
- Understanding self assembly of silica precursors using Monte Carlo simulations (I Shere and **A Malani**)
- 2017 Department of Chemical Engg., IIT Kanpur, India.
- Nanoporous materials for gas separation and storage (**A Malani**)
- 2016 Workshop on Recent Trends in Chemical Engineering, NIT Surat, India (**Invited**)
- Structure and dynamics of confined fluids (**A Malani**)
- 2014 AIChE Annual Meeting, Atlanta, USA.
- Influence of surface ions on adsorption of water on hydrophilic surface: Molecular simulation study (R Debbarma and **A Malani**)
- 2014 Molecular Modeling and Simulation of Sustainable Polymers and Nanocomposites, IIT Guwahati, India (**Invited**)
- Fundamentals of molecular modelling and application to silica polymerization (**A Malani**)
- 2014 Soft Matter - Young Investigator Meet, Pondicherry, India.
- Molecular level modeling of wetting behaviour and self assembly processes.
- 2013 Asian Conference on Colloid and Interface Science, North Bengal University, India.
- Float method: Measuring equilibrium and dynamic contact angles using molecular simulations (**A Malani** and G Rutledge)
- 2013 AIChE Annual Meeting, San Francisco, USA.
- Can dynamic contact angle be measured using molecular modeling? (**A Malani**, A Raghavanpillai, E Wysong and G Rutledge)
- 2013 Mumbai-Pune Soft Matter Meet, IIT Bombay, India.
- Molecular level modeling of equilibrium and dynamic contact angle phenomena (**A Malani**)
- 2012 Department of Chemical Engineering, University of Illinois at Chicago, USA.
- Molecular level modeling of wetting behaviour and self-assembly processes (**A Malani**)

- 2012 International Symposium on Contact Angle, Wettability and Adhesion, Quebec City, Canada
- Molecular modeling of three phase contact for static and dynamic contact angle phenomena (**A Malani**, A Raghavanpillai, E Wysong and G Rutledge)
- 2012 Department of Chemical Engineering, IIT Kanpur, India
- Molecular level modeling of wetting behavior and self-assembly processes (**A Malani**)
- 2012 Department of Chemical Engineering, IIT Kharagpur, India
- Molecular level modeling of wetting behavior and self-assembly processes (**A Malani**)
- 2012 Department of Chemical Engineering, IIT Hyderabad, India
- Molecular level modeling of wetting behavior and self-assembly processes (**A Malani**)
- 2011 AIChE Annual Meeting, Minneapolis, USA
- Molecular level modeling of three-phase contact for static and dynamic contact angle phenomena (**A Malani**, A Raghavanpillai, E Wysong and G Rutledge)
- 2011 Department of Chemical Engineering, IIT Bombay, India
- Molecular modeling of silica polymerization and interfacial water (**A Malani**)
- 2010 AIChE Annual Meeting, Salt Lake City, USA
- Molecular level modeling of three phase contact (**A Malani**, M Amat and G Rutledge)
 - Probing the mechanism of silica polymerization at ambient temperature using molecular simulations (**A Malani**, S Auerbach and P Monson)
- 2010 DuPont-MIT Alliance Symposium, MIT, USA
- Modeling surface properties of fluoropolymers (**A Malani** and G Rutledge)
- 2010 Department of Chemistry, University of Michigan, USA (**Invited**)
- Interfacial water and silica polymerization: Molecular simulation studies (**A Malani**)
- 2009 AIChE Annual Meeting, Nashville, USA
- Influence of hydrophilic surface specificity on structural properties of confined water (**A Malani**, K G Ayappa and S Murad)
 - Dynamics of water near mica surfaces (**A Malani** and K G Ayappa)
 - Water adsorption on mica: Redistribution and film growth (**A Malani** and K G Ayappa)
- 2009 Research Colloquium, Indian Institute of Science, Bangalore, India
- Structure and dynamics of interfacial and confined water (**A Malani**)
- 2008 NanoSikkim-III: Mechanics and Friction at Nanoscale, Sikkim, India
- Water structure and forces between hydrophilic surfaces (**A Malani** and K G Ayappa)
- 2008 Bangalore Area Statistical Mechanics Meeting, Bangalore, India
- Solvation and solubility of ions in nanopores (**A Malani**, K G Ayappa and S Murad)
- 2007 AIChE Annual Meeting, Salt Lake City, USA
- Solvation and solubility of ions in nanopores (**A Malani**, K G Ayappa and S Murad)
- 2006 Midwest Thermodynamics and Statistical Mechanics Conference, Akron, USA
- Effect of confinement on solubility of NaCl in water (**A Malani**, K G Ayappa and S Murad)

Oral Presentations From My Group

- 2018 Chemference, IIT Bombay, India
- How to synthesize a desired polymeric structure? (**I Shere** and A Malani)
 - Methane adsorption in multilayer frameworks (**A Sharma**, R Babarao, N Medhekar and A Malani)

- 2017 AIChE Annual Meeting, Minneapolis, USA
- Development of reaction ensemble Monte Carlo (REMC) algorithms to study the kinetics of silica polymerization (**I Shere** and A Malani)
- 2017 Research Scholar Symposium, IIT Bombay, India
- Kinetics studies of silica polymerization using reaction ensemble Monte Carlo (REMC) (**I Shere** and A Malani, 3 minute talk, **Received best oral presentation award**)
 - Competitive adsorption of ions at solid-liquid interface: Molecular simulation study (**S Adapa** and A Malani, **Received best oral presentation award**)
- 2016 Gordon Research Seminar, Holderness, NH, USA
- Understanding the adsorption of cations at mica-aqueous interface (**S Adapa** and A Malani)
- 2016 Research Scholar Symposium, IIT Bombay, India
- Study of kinetics of polymerization using reaction ensemble Monte Carlo (REMC) (**I Shere** and A Malani, **Received best oral presentation award**)
 - Performance of slipped polyimide covalent organic frameworks for CO₂:N₂ adsorption and separation (**A Sharma**, R Babarao, N Medhekar and A Malani)
- 2015 Chemference, IIT Hyderabad, India
- Effect of slipping on CO₂ adsorption in covalent organic frameworks (**A Sharma**, R Babarao, N Medhekar and A Malani)

Poster Presentations From My Group (list only those which have received awards with presenter name)

- 2018 Chemference, IIT Bombay, India.
- Adsorption of ions at solid-liquid interface (Sai Adapa)
- 2018 Research Scholar Symposium, IIT Bombay, India.
- Effect of slipping and functionalization on methane adsorption and separation performance of covalent organic frameworks (Abhishek Sharma)
- 2017 Vortex, ICT Mumbai, India.
- Water adsorption on solid surfaces: Molecular simulation study (S. Maity and D. Swami)
- 2017 ReSConAM, IIT Bombay, India.
- Effect of slipping in covalent organic frameworks on CO₂ adsorption and CO₂:N₂ separation (Abhishek Sharma)
- 2017 Research Scholar Symposium, IIT Bombay, India.
- Review on molecular dynamics simulations of lipid bilayers (Afroz Momin)
- 2016 Research Scholar Symposium, IIT Bombay, India.
- Understanding wetting behaviour of carbon nanotubes (Lakshay Gridhar)
- 2016 Gordon Research Seminar, Holderness, NH, USA.
- Understanding the adsorption of cations at mica-aqueous interface (Sai Adapa)
- 2015 Research Scholar Symposium, IIT Bombay, India.
- Monte Carlo (MC) simulation of silica polymerization of two, three, and four functional alkoxides (Inderdip Shere)

Students Advised

Post-Doctoral Associates:

- 1 Dr. Meena Singh, (PhD - ICT Mumbai)

Doctoral Students:

- 1 Inderdip Shere (Chem. Engg.), IIT Bombay
- 2 Sai Krishna (Chem. Engg.), IIT Bombay
- 3 Abhishek Sharma (Chem. Engg.), IITB-Monash Academy
- 4 Rabia Rahmani (CRNTS), Co-advised with Prof. Ajay Panwar
- 5 Afroz Momin (Chem. Engg.), Co-advised with Prof. Sameer Jadhav
- 6 Suvardhan Jogannadala (Chem. Engg.), IITB-Monash Academy

Graduate Students

- 1 Abhishek Thanvi (Dual Degree), IIT Bombay
- 2 Ravi Yemmadi (M.Tech.), IIT Bombay
- 3 Lakshya Gridhar (M.Tech.), IIT Bombay
- 4 Bablu Meghwal (M.Tech.), IIT Bombay

Undergraduate Students

- 1 Ahmed Murtuza Abbasi, IIT Bombay
- 2 Rousan Debbarma, IIT Bombay
- 3 Khushal Melana, IIT Bombay
- 4 Vishal Badri, IIT Madras
- 5 Sonam Kumari, MNIT Jaipur
- 6 Nakul Rampal, Manipal Inst. Tech., Manipal
- 7 Nikhil Rampal, Manipal Inst. Tech., Manipal
- 8 Dhananjay Swami, ICT Mumbai
- 9 Samdarishi Maity, ICT Mumbai.
- 10 Shobhit Chaturvedi, PIET, Nagpur
- 11 Sohan Ahmed, Manipal Inst. Tech., Manipal