

## **Arun Kumar Narayanan Nair**

*Ph.D. in Theoretical Physics (2006), Max Planck Institute, Germany*

### **Curriculum Vitae**

#### **PERSONAL DATA**

Name: Arun Kumar Narayanan Nair  
Date of birth: 7<sup>th</sup> June 1979  
Place of birth: Kerala, India  
Gender: Male  
Citizenship: Indian  
Languages: English (fluent), Hindi (fluent), Malayalam (fluent), German (beginner)  
Marital status: Married  
Spouse's name: Dr. Aparna Balakrishna  
Children: 2 daughters (Bhadra Arun & Lakshmi Nair)  
Permanent address: Valayamkode House,  
Karikode P.O., Kottayam District,  
Kerala, India. PIN – 686610  
Tel.: +91-4829-258091  
E-mail/Skype id: anarayanannair@gmail.com; anarayanannair  
ORCID ID: 0000-0002-2776-4006

#### **EDUCATION/PROFESSION**

04/16 – present: Scientist (R3), King Abdullah University of Science and Technology (KAUST), Kingdom of Saudi Arabia.  
04/14 – 04/16: Post-doc Fellow, KAUST, Kingdom of Saudi Arabia.  
11/10 – 03/12: Research Fellow, The University of Texas (UT) at Austin, USA.  
06/07 – 11/10: Post-doc, The University of North Carolina (UNC) at Chapel Hill, USA.  
04/06 – 08/06: Post-doc, Max-Planck-Institut für Kolloid- und Grenzflächenforschung (MPIKG), Potsdam, Germany.  
04/03 – 04/06: Ph.D. in Theoretical Physics (*magna cum laude/high honor*), MPIKG.  
11/99 – 07/02: Master of Science in Physical Chemistry (*first rank with distinction - 79.3%*), Mahatma Gandhi University, Kerala, India.  
07/96 – 03/99: Bachelor of Science in Chemistry (*first class - 76.1%*), Mahatma Gandhi University, Kerala, India.

#### **RESEARCH EXPERIENCE**

01/18 – present: *Simulations of adsorption and diffusion of byproducts formed by the peroxide-induced cross-linking of polyethylene*, KAUST, Thuwal (Funded by The Dow Chemical Company under Award RGC/3/3560-01).

- 04/17 – 03/19: *Simulations and theory of pH-Responsive Polyelectrolytes*, KAUST, Thuwal (Funded by the KAUST Office of Sponsored Research (OSR) under Award URF/1/2993-01).
- 04/14 – 03/18: *Simulations of shale media: Adsorption and flow*, KAUST, Thuwal (Funded by Saudi Aramco under Award RGC/3/2053-01).
- 11/10 – 03/12: *Self-Assembly of Semiflexible-Flexible Block Copolymers*, UT, Austin.
- 06/09 – 11/10: *Simulation of Self-Healing Polymer Networks*, UNC, Chapel Hill (Funded by National Science Foundation (NSF)).
- 06/07 – 06/09: *Simulation of Shear Forces Between Charged Polymer Brushes*, UNC, Chapel Hill.
- 04/03 – 04/06: *Molecular Dynamics Simulations of Polyelectrolyte Brushes*, MPIKG, Potsdam.
- 11/01 – 02/02: *Theory of Breaking of a Weak Link in a Stiff Ring Polymer*, Indian Institute of Science, Bangalore, India.

### COMPUTER SKILLS

- Programming languages: Experience with FORTRAN77/90 and C. Knowledge of C++, perl, UNIX scripts (tcsh etc.).
- Software packages/Parallel computing: Experience with Mathematica, Matlab, Grace, RasMol, VMD, DL-POLY, LAMMPS, Towhee, RASPA, Gromacs, Medea, self-consistent-field theory (SCFT) simulation. Experience using Message Passing Interface (MPI).
- Miscellaneous: Experience with Linux, Unix and Windows operating systems.

### **PUBLICATIONS/PROJECTS (google scholar) (citations:500+, h-index:10+)** **Publications as corresponding author (work at KAUST, Kingdom of Saudi Arabia)**

- [1] Yang, Y.; Nair, A. K. N.; Sun, S.; Sun, Y.; Van Dun, J.; Kjellqvist, J. (2019) Studies of Diffusion of Byproducts Formed by the Peroxide-Induced Cross-Linking of Polyethylene. Jicable'19, Versailles, France.
- [2] Yang, Y.; Nair, A. K. N.; Sun, S. (2019) Adsorption and Diffusion of Methane and Carbon Dioxide in Amorphous Regions of Cross-Linked Polyethylene: A Molecular Simulation Study. Industrial & Engineering Chemistry Research DOI: 10.1021/acs.iecr.9b00690 (IF: 3.2, Times Cited: 1)
- [3] Yang, Y.; Che Ruslan, M.F.A.; Nair, A. K. N.; Sun, S. (2019) Effect of Ion Valency on the Properties of the Carbon Dioxide–Methane–Brine System. Journal of Physical Chemistry B 123, 2719 (IF: 3.2, Times Cited: 2)
- [4] Li, Y.; Nair, A. K. N.; Kadoura, A.; Yang, Y.; Sun, S. (2019) Molecular Simulation Study of Montmorillonite in Contact with Water. Industrial & Engineering Chemistry Research 58, 1396 (IF: 3.2, Times Cited: 2)
- [5] Yang, Y.; Nair, A. K. N.; Sun, S. (2017) Molecular Dynamics Simulation Study of Carbon Dioxide, Methane, and Their Mixture in the Presence of Brine. Journal of Physical Chemistry B 121, 9688 (IF: 3.2, Times Cited: 7)
- [6] Nair, A. K. N.; Jimenez, A. M.; Sun, S. (2017) Complexation Behavior of Polyelectrolytes and Polyampholytes. Journal of Physical Chemistry B 121, 7987 (IF: 3.2, Times Cited: 6)
- [7] Kadoura, A.; Nair, A. K. N.; Sun, S. (2017) Molecular Simulation Study of Montmorillonite in Contact with Variably Wet Supercritical Carbon Dioxide. Journal of Physical Chemistry C, 121 (11), 6199 (IF: 4.8, Times Cited: 18)

- [8] Kadoura, A.; Nair, A. K. N.; Sun, S. (2016) Molecular Dynamics Simulations of Carbon Dioxide, Methane, and their Mixture in Montmorillonite Clay Hydrates. *Journal of Physical Chemistry C*, 120 (23), 12517 (IF: 4.8, Times Cited: 30)
- [9] Kadoura, A.; Nair, A. K. N.; Sun, S. (2016) Adsorption of carbon dioxide, methane, and their mixture by montmorillonite in the presence of water. *Microporous and Mesoporous Materials*, 225, 331 (IF: 3.5, Times Cited: 36)
- [10] Nair, A. K. N.; Uyaver, S.; Sun, S. (2014) Conformational Transitions of a Weak Polyampholyte. *The Journal of Chemical Physics*, 141(13), 134905 (IF: 3.1, Times Cited: 15)

#### **Publications from work at Mahatma Gandhi University, Kerala, India**

- [11] Balakrishna, A.; Kumar, N. A. (2012) Preliminary Studies on Siderophore Production and Probiotic Effect of Bacteria Associated with the Guppy, *Poecilia reticulata* Peters, 1859. *Asian Fisheries Science* 25, 193 (Times Cited: 3)
- [12] Theory of Breaking of a Weak Link in a Stiff Ring Polymer (Times Cited: 1)  
M.Sc. Thesis (2002) done with Prof. K.L. Sebastian, Indian Institute of Science, India.

#### **Publications from work at UT, Austin, Texas, U.S.A**

- [13] Ganesan, V.; Kumar, N. A.; Pryamitsyn, V. (2012) Blockiness and Sequence Polydispersity Effects on the Phase Behavior and Interfacial Properties of Gradient Copolymers. *Macromolecules* 45, 6281 (IF: 5.1, Times Cited: 35)
- [14] Kumar, N. A.; Ganesan, V. (2012) Self-Assembly of Semiflexible-Flexible Block Copolymers. *The Journal of Chemical Physics* 136, 101101 (IF: 3.122, Times Cited: 36)  
*One of the editor's choice papers for the year 2012*

#### **Publications from work at UNC, Chapel Hill, NC, U.S.A.**

- [15] Cai, L.; Stukalin, E.; Kumar, N. A.; Leibler L.; Rubinstein, M. (2013) Self-Healing of Unentangled Polymer Networks with Reversible Bonds. *Macromolecules* 46, 7525 (IF: 5.1, Times Cited: 134)  
*One of the journal's top 5 most read articles in Sep-Oct 2013 (1-month basis)*

#### **Publications from work at MPI of Colloids and Interfaces, Potsdam, Germany**

- [16] Kumar, N. A.; Seidel, C. (2007) Interaction between Two Polyelectrolyte Brushes. *Physical Review E* 76, 020801(R) (IF: 2.4, Times Cited: 36)
- [17] Kumar, N. A. (2006) Molecular Dynamics Simulations of Polyelectrolyte Brushes. Ph.D. Thesis, University of Potsdam, Potsdam, Germany
- [18] Seidel, C.; Kumar, N. A. (2006) Molecular Dynamics Simulations of Polyelectrolyte Brushes. NIC Symposium 2006, NIC series, John von Neumann Institute for Computing, Jülich, 32, 253
- [19] Kumar, N. A.; Seidel, C. (2005) Polyelectrolyte Brushes with Added Salt. *Macromolecules* 38, 9341 (IF: 5.1, Times Cited: 91)
- [20] Ahrens, H.; Forster, S.; Helm, C. A.; Kumar, N. A.; Naji, A.; Netz, R. R.; Seidel, C (2004) Nonlinear Osmotic Brush Regime: Experiments, Simulations and Scaling Theory. *Journal of Physical Chemistry B* 108, 16870 (IF: 3.7, Times Cited: 73)

#### **RESEARCH GRANT PROPOSALS**

- Nair, A. K. N.; Sun, S “Modeling of Methane and Peroxide By-Product Release for Polyolefin-Based Crosslinked Cables”, funded by Dow, Jan 1, 2018 – Dec 31, 2020. Grant amount: US\$ 1 million.

- Nair, A. K. N.; Sun, S; Ganesan, V. “pH-Responsive Polyelectrolytes: Monte Carlo Simulation and Self-Consistent Field Theory”, funded by KAUST’s Competitive Research Grants (CRG) program, April 1, 2017 – March 31, 2019. Grant amount: US\$ 0.4 million.
- Uyaver, S.; Nair, A. K. N.; Sun, S. Simulation of Lubrication by Mixed Polymer Brushes, Submitted, Tubitak, Ankara, Turkey, 2015.
- Nair, A. K. N.; Sun, S. Investigation of adsorption and desorption of gas in shale, Submitted to Baker Hughes.
- Nair, A. K. N.; Sun, S. Molecular Simulations of Fluid-Rock Interaction, Submitted to Aramco.

## **PRESENTATIONS/WORKSHOPS/TEACHING EXPERIENCE**

- Given lecture (1 class of 1.30 hours) on *Molecular Simulations: Applications to graduate students of Physical Sciences and Engineering (PSE)*, 2019, KAUST.
- Given talk titled *Molecular Simulation Study of Swelling Clays*, May 17, 2018, New Orleans, USA.
- Given talk titled *Molecular Simulation of Gas Adsorption and Diffusion in Shale Media*, Feb. 09, 2017, Saudi Aramco, Dhahran.
- Given lectures (2 classes of 1.30 hours each) on *Molecular Simulations to graduate students of Physical Sciences and Engineering (PSE)*, 2016, KAUST.
- Given talk on *Adsorption of carbon dioxide, methane, and their mixture by montmorillonite in the presence of water*, Dec. 21, 2015, Saudi Aramco, Dhahran.
- Given lectures (4 classes of 1.30 hours each) on *Molecular Dynamics and Monte Carlo Simulations to graduate students of PSE*, 2014, KAUST.
- Given soundbite titled *Simulations of Self-Healing Polymer Networks*, 12th May 2010, Triangle Soft Matter Workshop, Duke University, Durham, North Carolina, U.S.A.;
- *Simulation of Shear Forces Between Charged Polymer Brushes*, 8th May 2009, Triangle Soft Matter Workshop, North Carolina State University, North Carolina, U.S.A.
- Given talk titled *Simulations of Self-Healing Polymer Networks*, 18th March 2010, APS March Meeting 2010, Portland, Oregon, U.S.A.
- Attended lectures on *Polymer Physics* during 2007-08, offered by Prof. Michael Rubinstein at Department of Chemistry, University of North Carolina, U.S.A.
- Given talk titled *Molecular Dynamics Simulations of Polyelectrolyte Brushes*, 16th February 2007, Laboratory of Physics, Helsinki University of Technology, Finland; 1st June 2006, Department of Chemistry, University of North Carolina, U.S.A.
- Attended workshop on *Introduction to Programming and Using the IBM Supercomputer Jülich Multiprocessor (JUMP)* at Research Centre Jülich, from 4 - 5 July 2005 organized by Zentralinstitut für Angewandte Mathematik, Jülich, Germany.
- Assisted in teaching *Computer Simulations* course (Oct. 2004 - Feb. 2005), within the frame work of International Max Planck Research School (IMPRS) on Biomimetic Systems, Potsdam, Germany (<http://www.imprs.org/>).
- Obtained credit points in various semester courses, e.g. *Polymer Physics*, *Protein Folding*, and attended student seminars on *Theory of Soft and Biomatter*, offered by IMPRS on Biomimetic Systems during 2003 - 05.
- Presented poster titled *Polyelectrolyte Brushes with Added Salt*, April 24th 2004, on the occasion of IMPRS evaluation, Potsdam, Germany. Given talks at internal department workshops MPIKG (2003 - 05), UNC (2007 - 09).

### **Presentations of my work by co-authors**

- Sun, S.; Nair, A. K. N. *Multi-scale fluid flow & transport through porous media*, June 18-22, 2017, Frankfurt, Germany.
- Uyaver, S.; Nair, A. K. N.; Sun, S. *Monte Carlo simulations of a weak polyampholyte*, May 10-14, 2015, Český Krumlov, Czech Republic.
- Ganesan, V.; Kumar, N. A. *Self-assembly of semiflexible-flexible block copolymers*, 29th Feb 2012, APS March Meeting 2012, Boston, Massachusetts, U.S.A.
- Rubinstein, M.; Kumar, N. A.; Stukalin, E.; Leibler L. *Autonomous Self-Healing in Polymer Networks*, 30th Aug 2010, Polymer Networks Group 20<sup>th</sup> Conference 2010, Goslar, Germany

#### **Graduate teaching assistantship at KAUST**

- Assisting Mr. Mohd Fuad Anwari Che Ruslan with his Ph.D. thesis, PSE, KAUST, 2018-present (1 joint publication).
- Assisting Mr. Yafan Yang with his Ph.D. thesis, PSE, KAUST, 2016-present (4 joint publications).
- Assisting Mr. Yiteng Li with his Ph.D. thesis, PSE, KAUST, 2016-present (1 joint publication).
- Assisted Mr. Ahmad Kadoura with his Ph.D. thesis, PSE, KAUST, 2014-2016 (4 joint publications).
- Assisted Mr. Arturo Martinez Jimenez with his M.Sc. thesis, PSE, KAUST, 2015-2016 (1 joint publication).
- Assisted Mr. Xiaolin Fan with his project “Apparent Permeability in Shale Media”, PSE, KAUST, 2014.
- Assisted Ms. Sahar Amir with Monte Carlo simulations for determining the bulk chemical potential of high density fluids, PSE, KAUST, 2014.

#### **AWARDS/HONORS**

- Magna cum laude (high honor) for Ph.D. in Theoretical Physics.
- First rank in M.Sc. Physical Chemistry.
- Passed Graduate Aptitude Test in Engineering in 2002.
- Qualified National Eligibility Test (NET) in 2002 conducted by University Grants Commission and Council for Scientific and Industrial Research, India (NET qualifiers are eligible for lectureship in Indian universities).
- Merit Certificate in Std. X.
- Played in the cricket team for the chemistry department during the inter-departmental cricket tournament, February 2000, at Mahatma Gandhi University and stood first.

#### **JOURNAL/PROPOSAL REVIEW**

- J. Phys. Chem., Industrial & Engineering Chemistry Research, Energy & Fuels (American Chemical Society)
- US Dept. of Energy
- Journal of Rock Mechanics and Geotechnical Engineering, Elsevier
- Science China Technological Sciences, Springer

#### **PAST POST-DOC/RESEARCH OFFERS RECEIVED**

- 2016: KAUST, Kingdom of Saudi Arabia (accepted) (Prof. Shuyu Sun)
- 2013: KAUST, Kingdom of Saudi Arabia (accepted) (Prof. Shuyu Sun)

2013: University of Crete, Greece  
2012: Université libre de Bruxelles, Belgium  
2012: Georgia Institute of Technology, USA  
2010: UT at Austin, USA (accepted) (Prof. Venkat Ganesan)  
2007: UNC at Chapel Hill, USA (accepted) (Prof. Michael Rubinstein)  
2006: Helsinki University of Technology, Finland  
2006: University of Ottawa, Canada  
2006: University of Massachusetts, Amherst, USA  
2006: MPIKG, Germany (accepted) (Prof. Reinhard Lipowsky)

**COUNTRIES VISITED**

Germany, U.S.A., Belgium, Austria, Italy, Finland, Kingdom of Saudi Arabia

**SCIENTIFIC/PROFESSIONAL MEMBERSHIPS**

American physical society