

Dr. Parimal Kar

EDUCATION

- Ph.D. (Physics/Computational Biophysics), Michigan Technological University, USA
- M.Sc. (Physics), Indian Institute of Technology Bombay, India
- B. Sc. (Physics), University of Calcutta, Kolkata, India

WORK EXPERIENCE

- Ramalingaswamy Fellow, BSBE, IIT Indore (2016 -).
- Visiting Research Associate, Michigan State University, USA (2012 – 2016).
- Guest Scientist, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany (2010 – 2012).
- Visiting Scholar, Forschungszentrum Jülich, Germany (02/2008 – 07/2008).
- Graduate Intern, Center for Nonlinear Studies (CNLS), Los Alamos National Laboratory, NM, USA (06/2009 – 12/2009).
- Visiting Student, Forschungszentrum Jülich, Germany (05/2007 – 08/2007).

AWARDS AND FELLOWSHIPS

- Ramalingaswamy Fellowship, DBT, India (2015).
- Postdoctoral Independent Career Potential Award, Michigan State University, East Lansing, MI, USA (2014).
- IGRTG Postdoctoral Fellowship, German Research Foundation (2011).
- Biotechnology Research Center Travel Grant Award, Michigan Technological University (2007).
- Visiting Student Fellowship, Forschungszentrum Jülich, Germany (2006, 2007, 2008).

MEMBERSHIP TO PROFESSIONAL ORGANIZATION

- Member, Biophysical Society (BPS).
- Member, American Chemical Society (ACS).

RESEARCH

- Development and applications of coarse-grained (CG) and multiscale all-atom/coarse-grained (AA/CG) methods for biomolecules (proteins, nucleic acids, and carbohydrates) and mechanistic study of large bimolecular systems.
- Multiscale modeling of biomolecular recognition, protein-ligand interactions.
- Protein–membrane interactions
- Free energy simulations and enhanced sampling methods
- Modeling host-pathogen interactions in infectious diseases and innate immune response
- Interaction of carbohydrates (glycans) with proteins and membrane

PUBLICATIONS

- H. Memczak, D. Lauster, P. Kar, S. Di Lella, R. Volkmer, V. Knecht, A. Hermann, E. Ehrentreich-Förster, F. F. Bier, W. F. M. Stöcklein. 2016. Anti-Hemagglutinin Antibody Derived Lead Peptides for Inhibitors of Influenza Virus Binding. *PLoS One*, 11 (7), e0159074.
- S. Sengupta, R. Lingnurkar, T. Carey, M. Pomaville, P. Kar, M. Feig, C. Wilson, J. G. Knott, D. N. Arnosti, R. W. Henry. 2015. The Evolutionary Conserved C-terminal Domain in the Mammalian RB Family Serves as a Dual Regulator of Protein Stability and Transcriptional Potency. *J. Biol. Chem.* 290, 14462–14475.
- P. Kar and M. Feig. 2014. Recent Advances in Transferable Coarse-Grained Modeling of Proteins, *Advances in Protein Chemistry and Structural Biology*, 96, 143–180.
- P. Kar, S. M. Gopal, A. Panahi, Y.-M. Cheng, and M. Feig. 2014. Transferring the Coarse-Grained Force Field PRIMO to the Membrane Environment: Simulation of Proteins and Helix-Helix Association, *J. Chem. Theory Comput.*, 10 (8), 3459–3472.
- P. Kar, S. M. Gopal, Y.-M. Cheng, A. Predeus, and M. Feig. 2013. PRIMO: A Transferable Coarse-Grained Force Field for Proteins, *J. Chem. Theory Comput.*, 9 (8), 3769–3788.
- P. Kar, R. Lipowsky, and V. Knecht. 2013. Importance of Polar Solvation and Configurational Entropy for Design of Antiretroviral Drugs Targeting HIV-1 Protease, *J. Phys. Chem. B*, 117 (21), 5793–5805.
- P. Kar and V. Knecht. 2012. Energetics of Mutation Induced Changes in Potency of Lersivirine against HIV-1 Reverse Transcriptase, *J. Phys. Chem. B*, 116(21), 6137–6149.
- P. Kar and V. Knecht. 2012. Mutation-Induced Loop Opening and Energetics for Binding of Tamiflu to Influenza N8 Neuraminidase, *J. Phys. Chem. B*, 116(22), 6269–6278.
- P. Kar and V. Knecht. 2012. Energetic Basis for Drug Resistance of HIV-1 Protease Mutants against Amprenavir, *J. Comput.-Aided Mol. Des.* 26(2), 215–232.
- P. Kar and V. Knecht. 2012. Origin of Decrease in Potency of Darunavir and Two Related Antiviral Inhibitors against HIV-2 Compared to HIV-1 Protease, *J. Phys. Chem. B*, 116 (8), 2605–2614.
- P. Kar, R. Lipowsky, and V. Knecht. 2011. Energetics of Cross-reactivity of Diels-Alderase Antibody 1E9 and Its Variants with Steroid, *Proceedings of the CBSB 2011*, IAS Publication Series, Vol. 8(2011), 57–60.
- P. Kar, R. Lipowsky, and V. Knecht. 2011. Importance of Polar Solvation for Cross-reactivity of Catalytic Antibody and Its Variants with Steroids, *J. Phys. Chem. B* 115(23), 7661–7669.
- P. Kar, W. Nadler, U. H. E. Hansmann. 2009. Microcanonical Replica Exchange Molecular Dynamic Simulation of Proteins, *Phys. Rev. E* 80, 056703 (Selected for the December 1, 2009 issue of *Virtual Journal of Biological Physics Research*).
- P. Kar, M. Seel, T. Weidemann, and S. Höfinger. 2009. Theoretical Mimicry of Biomembrane, *FEBS Letters* 583(12), 1909–1915.
- P. Kar, Y. Wei, U. H. E. Hansmann, and S. Höfinger. 2007. Systematic Study of Boundary Composition in Poisson-Boltzmann Calculations, *J. Comput. Chem.* 28(16), 2538–2544.

- P. Kar, M. Seel, U. H. E. Hansmann, and S. Höfner. 2007. Dispersion Terms and Analysis of Size- and Charge-Dependence in an Enhanced Poisson-Boltzmann Approach, *J. Phys. Chem. B*, 111(30), 8910–8918.
- P. Kar, M. Seel, U. H. E. Hansmann, and S. Höfner. 2007. Comparing Semiempirical versus Classical Charge Assignments in Biomolecules and Their Effect on Electrostatic Potentials. *NIC Publication Series*, 36, 155–158.
- P. Kar, M. Seel, U. H. E. Hansmann, and S. Höfner. 2007. Algorithmic Refinements to an Enhanced Poisson-Boltzmann Approach Used in Biomolecular Simulations. *NIC Publication Series*, 36, 173–176.
- P. Kar, Y. Wei, U. H. E. Hansmann, and S. Höfner. 2006. The Influence of Molecular Surface Composition on the Outcome of Poisson-Boltzmann Calculations Performed to Obtain Solvation Free Energies. *NIC Publication Series*, 34, 205–209.

RESEARCH OPPORTUNITIES

The Kar's Lab is looking for two PhD students in the broader areas of computational biophysics. Students should be self-motivated. Some experience with molecular simulation is an advantage, but not essential. Motivated students from Physics, Chemistry, and Biosciences/Biotechnology departments are strongly encouraged to apply through IIT Indore PhD programme or can directly send their CV and cover letter to parimal@iiti.ac.in.