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Recent publications	• **S. Roy***, T. M. Ataol and F. Müller-Plathe: Molecular dynamics simulations of heptyl phosphonic acid: a potential polymer component for fuel cell polymer membrane, J. Phys. Chem. B, 112 (2008), 7403-7409 • **S. Roy** and M. Springborg: Structural and Electronic Properties of Indium Phosphide Nanotubes, J. Phys. Chem C; 113(2009), 81-86 • **S. Roy***, D. Markova, A. Kumar, M. Klapper and F. Müller-Plathe, Morphology of phosphonic-acid-functionalized block copolymers studied by dissipative particle dynamics, Macromolecules, 42 (2009), 841–848 • Prithvi Raj Pandey and **S. Roy***, Early Stages of Unwinding of Zwitterionic -Helical Homopolymeric Peptides, Chem. Phys. 514(2011), 330-335 • P.R.Pandey, **S.Roy***, Head group mediated water insertion in DPPC bilayer, J. Phys. Chem. B, 115(2011), 3155–3163 • Souvik Chakraborty, **S. Roy***, Structural, Dynamical, and Thermodynamical Properties of Carbon Nanotube Polycarbonate Composites: A Molecular Dynamics Study, J. Phys. Chem. B, 116 (2012), pp 3083–3091