A one day theme meeting on “Applications of Molecular Modeling in Separation Processes” AMMSP2015 was organized at C Block Auditorium, BARC, Mumbai on January, 16, 2015. The meeting was organized by Chemical Engineering Division, BARC in association with Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE). The welcome address was given by Shri K.T. Shenoy, Head, ChED and Convener, AMMSP2015. In his speech Dr. S. L. Chaplot Director, Physics Group and Chief Guest for the meeting, stressed the needs of the multidisciplinary approach while solving practical problems. The meeting was inaugurated by Prof. Swapan K Ghosh, Raja Ramanna Fellow. Prof Ghosh gave an inaugural lecture on “Perspectives on theory and modeling of materials and processes”. He emphasized on the synergy between theory, computation and experiment in all branches of sciences and engineering for best conceptualization and successful implementation of a research programme and suggested a requirement of a suitable forum for hand shaking between modelling and experiment. The proceedings of the meeting were released by Dr. Chaplot. The vote of thanks was delivered by Dr. Sk. Musharaf Ali, Head, LSS/ChED and Secretary, AMMSP2015. Presentations on various aspects of molecular modeling included application of the computational tool for selection of suitable ligand for the extraction of metal ion, An/Ln separation and isotope separation; design of low toxic drug molecules, nano particles and catalysts; fluid flow in nano tubes and metal organic framework for separation of fluids; thermodynamics of molten salt and Carbon nanotubes based adsorbents for An/Ln separation were presented. Experts from various institutes like ICT-Mumbai, IICT- Hyderabad, IIT-Mumbai and BARC made the presentation on these various aspects of the theme meeting. In the concluding session, a panel discussion was conducted where Prof. Dilip Maity, Associate Dean, HBNI stressed the needs of the platform where the modeling group and experimentalists can come together to solve the complex chemical separation processes of departmental needs.