	14.11.2013 Thursday	15.11.2013 Friday	16.11.2013 Saturday	17.11.2013 Sunday	18.11.2013 Monday	19.11.2013 Tuesday
9:00		Fluids - Methane Adsorption in Single Wall Carbon Nanotubes - N-Heptane Adsorption on Silicalite - Density & Speed of Sound calculation of CO2 - Henry Constants of various gases in Ethanol Laboratory 304	L.R. Tagirov Mesoscopic materials: getting functionality by manipulating wave functions		Reports of participants Laboratory 304	Self training Laboratory 304
10:00	arrival REGISTRATION		V.V. Ryazanov Applications of SFS Josephson junctions in superconducting digital and quantum electronics Lecture Hall 110			
11-00		coffe break	coffe break		coffe break	coffe break
11:15		Phonon in MedeA 2.14 - Vibrational properties of SiO2 (Stishovite) - LO-TO splitting - IR/Raman spectra Laboratory 304	Polymers - Diffusion on N2 in PE and PEX - Polymer Property Prediction using Correlations Laboratory 304		Reports of participants Laboratory 304	Closing
13:00	lunch	lunch	lunch		lunch	
14:00	Opening workshop Introduction Lecture Hall 110	G. Logvenov MBE based rational design of multicomponent layered oxides Lecture Hall 110	Electronic Transport in MedeA® - Seebeck coefficient of Bi2Te3 - Anisotropic conductivity of MoS2 thin films Laboratory 304		D.A. Tayurskii Computer design of new materials - from atomic scale to macroscopic devices Laboratory 304	
15:00	Building - From Databases to Structures - Amorphous Films - Surfaces/Super cells/Molecules - Docking in Zeolites Laboratory 304	Industrial use of computer modeling for material research by MedeA® software platform Lecture Hall 110			Round table "Prospects of development of multi-scale modeling " Laboratory 304	departure
16:00			NMR properties - Chemical shifts and electric field gradients of L-Alanine Laboratory 304			
17:00	Excursion					

Workshop

Lecture