

Area Seminar

Title	Theoretical study on the Aluminium Nuclear Magnetic Resonance spectroscopy
Date and Time	20/01/2011 16:00:00
Speaker	Chengbin Li
Area	WuHan Institute of Mathematics and Physics(WIMP), WuHan, China
Venue	Theoretical Physics
	Room No. 469
Abstract	<p>In my talk, I will introduce our semi-empirical molecular mechanical study on the Al Nuclear Magnetic Resonance (NMR) spectroscopy of zeolites. In this procedure, we consider classical molecular mechanics to describe the zeolite and use quantum mechanics to study the dynamics in the active Al sites. I will present our theoretical results and compare them with other available theoretical and the experimental results. I will also show that a partial identification of Al sites in the zeolite framework is possible.</p>