

Division of Material Chemistry	Research field	Theoretical Chemistry	Lab. ID MC03
Laboratory web site	<a href="http://chem.s.kanazawa-u.ac.jp/theo/index.html">http://chem.s.kanazawa-u.ac.jp/theo/index.html</a>		
Research subjects			
<p>The study covers the static or dynamic structural investigation of materials such as the disordered crystals, hydrogen bonded crystals, and liquid crystals, by means of solid-state NMR measurements and quantum chemical calculations. We develop the analysis methods of solid-state NMR for the study of physical properties and highly-precise analysis methods of molecular dynamics. To analyze the static and dynamic properties of molecules and clusters, we are also developing new approach in quantum chemical calculation.</p>			
Master/Doctor course: Education policy, curriculum, typical activity in the laboratory			
<p>We give the student the choice of experiment group or calculation group.  Students in the experiment group study the physical properties of various materials, e.g. proton conductor, functional polymer, mesoporous material and other materials, by using mainly solid-state NMR. Other measurements, e.g. thermal measurement, electrical conductivity, are employed as necessary.  Students in the calculation group study physical properties by using quantum-chemistry calculation. The students may acquire coding to use computer.  All students in our laboratory read textbook of quantum mechanics in turns once a week.</p>			
Daily life in the laboratory, etc.			
<p>Students in our laboratory mainly perform seminars and researches.  The seminars are performed at certain time, while the researches are performed in line with life-style of each student.  We often have drinking party to exchange among the students and teachers and to raise our motivation for study.  (D2)</p>			
Message or comments by the laboratory faculty staffs			
<p>In our laboratory, we hope the students to not only in line with direction by the faculties, but also in exchanging opinions with each other.  Since, it is many what are known by only those who actually perform the experiments and calculation in proceeding with the research, equal exchanges of opinions are important.  Of course, although the faculties often teach the students initially, let's develop the research themes to more interesting things by discussion with each other.</p>			
Recent Master theses in these 3 years (+ more if appropriate)			
year.month	Thesis title (including English translation of Japanese thesis title)		
2017.9	Spin state of electron correlation terms in the MP2 method		
2017.9	Spin-Component-Scaled approximation for second-order electron propagator method		
2017.3	Local structure and dynamics of imidazole in proton conducting composite PVPA/xIm ( $x \geq 2$ )		
2016.3	Carbon-Carbon distance determination using solid-state two-dimensional exchange NMR		
2016.3	Molecular Motion and Proton Conductivity in Alginic Acid-Imidazole Composite		
2016.3	Structural Change and Proton Conductivity of Imidazolium Sebacate Crystal		
2015.9	Structure and Activity Relationships in Ferredoxin -NADP <sup>+</sup> - Reductase by Molecular Dynamics Simulation		
2015.3	Local Structure and Proton Conductivity of Imidazolium Hydrogen Malonate Crystal		
2014.3	Theoretical Studies for Proton Transfer in Imidazole		
2014.3	Investigation of Orientational Order and Dynamics of Hydrogen Bonded Liquid Crystals		
2013.3	Local Structure Analysis of In-doped ZnO Crystal by EFG tensor Calculations		
2013.3	Local Dynamics of Water in BSA (Bovine Serum Albumin) Crystal by Solid-State Deuterium NMR		
2013.3	Analysis of Water Dynamics and Liquid-Liquid Transition in the Pores of Mesoporous Silica by Deuterium NMR		
2013.3	Behavior of Small Molecules in Oriented Structure of Liquid Crystal and its Influence on Physical Property		
2013.3	Local Dynamics of Hydration Water in Hen Egg White Lysozyme using Solid-State NMR		
Recent Doctoral theses in these 3 years (+ more if appropriate)			
year.month	Thesis title (including English translation of Japanese thesis title)		
2017.3	Theoretical study of intermolecular proton transfer using diabatic potential		
2016.9	Phase transition and dynamics of water confined in nanoscale spaces		
2016.3	Molecular Orientation and Phase Transition of 7CB-n-heptane Binary System		
2013.9	Analysis of Local Structure and Molecular Motion of Proton-Conductive Imidazolium Hydrogen Succinate Crystal using Solid-State NMR		

Laboratory mail address

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