

**University of Puerto Rico**  
**Río Piedras Campus**  
**Faculty of Natural Sciences, Department of Physics**  
**Graduate Programme**

**Title:** Advanced Topics in Chemical Physics: Molecular Liquids.

**Code:** PHYS 8996

**Number of Credits:** 3

**Number of Hours** 3 hours of classroom lecture per week

**Prerequisites:** Permission of the Graduate Committee

**Effective date of the syllabus** Second Semester, 2022-2023 academic year

**Instructor** Lutful Bari Bhuiyan  
Office Natural Sciences II, C-350  
Class period: Por Acuerdo  
Office hours: Mondays and Wednesdays, 8 am – 10 am, 2 pm – 3.30 pm  
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### Description

Basic concepts ---- physical characteristics of a liquid compared to that of a solid or a gas. General properties of liquids, Experimental information about liquid structure ---- the structure factor, relation between the structure factor and the radial distribution function. Distribution function theory of structure. Relationship between force equation and structure, thermodynamics of liquids, the pair potential and structure, theories of liquids and simulation of liquid structure and thermodynamics through machine simulations, charged fluids.

### Objectives

After the completion of this course the student

- will learn the basic concepts of liquids and the experimental techniques of obtaining information about liquid structure and thermodynamics.
- will be capable of appreciating the statistical mechanics used in the description of classical fluids.
- will have the required background to understand and perform numerical calculations using programming languages to calculate structure factors and radial distribution functions of simple liquids
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### Course Contents

- **Week 1:** Basic concepts of the liquid state in relation to the solid and gaseous states of matter. Experimental information about structure, the structure factor  $S(q)$  obtained from diffraction probes. Relationship between  $S(q)$  and the pair correlation function  $g(r)$ .

- **Week 2,3,4:** The statistical mechanical distribution function theory of structure, energy, and pressure in a fluid..
- **Week 5,6:** Forces and structure . The pair potential  $u(r)$  and the potential of mean force  $U(r)$ . Extracting the structure from a knowledge of  $u(r)$ .
- **Week 7,8:** Theories of liquids and simulation of liquid structure through numerical simulations. The Ornstein-Zernike relation relating the total and direct correlation functions.
- **Week 9-10:** Charged fluids. The classical Debye-Hückel (DH) theory of structure and thermodynamics of dilute electrolytes. The Debye-Hückel limiting law (DHLL).
- **Week 10-11:** The Poisson-Boltzmann (PB) theory (non-linear) of electrolytes. The symmetric Poisson-Boltzmann (SPB) theory. Numerical solution.
- **Week 12-13:** Statistical Mechanical theories of electrolytes, the mean spherical approximation (MSA) and the hypernetted chain (HNC) theory
- **Week 14-15:** Statistical Mechanical theories of electrolytes (contd) – the modified Poisson-Boltzmann (MPB) theory.

### **Instructional Strategy**

The contents of the course will be offered in the form of lectures with emphasis in examples of applications to different branches of Condensed Matter Physics. The students are trained to apply the statistical mechanical techniques learnt to simple physical situations and setting up the problem mathematically, which is then solved using standard mathematical methods. A fair part of the lecturing effort is thus dedicated to the demonstration of solution of problems of kinetic theory, classical and quantum gases.

### **Minimum Facilities Required**

Traditional lecture room, High speed computers with broad band internet connection for the COVID situation.

### **Student Evaluation**

This will be based on classroom participation, assignments, presentations, ability to write numerical codes (using common programming languages) to calculate the structure and thermodynamics of simple liquids and then present results in class.

## **Grading System**

The student completing the course work will be graded according to the standard scale A to F.

## **Text**

*Theory of Simple Liquids*, J. –P. Hansen and I. R. McDonald, Academic Press, 1990,  
ISBN 0-12-323852-8

## **Bibliography**

*An Introduction to Statistical Mechanics*, Terrell L. Hill, Dover Publications, 1987,  
ISBN 978 0486652429

*Statistical Mechanics*, Donald A. McQuarrie, University Science Books, 2000,  
ISBN 978 1891389153

*An Introduction to the Liquid State*, P. A. Egelstaff, Oxford Science Publication,  
ISBN 0 19 8510128

*Chemical Physics of Liquids*, N. H. March, Gordon and Breach, 1990,  
ISBN 2-88124-722-9

**Additional learning resources** Wikipedia, Research article references to be given in class.

## **Rights of Students with Disabilities**

UPR complies with all federal and state laws and regulations regarding discrimination, including the Americans with Disabilities Act 1990 (ADA) and the Commonwealth of Puerto Rico Law 51. Students receiving services through Rehabilitaci3n Vocacional must contact the professor at the beginning of the semester in order to plan for a reasonable accommodation and any required support equipment according to the recommendations given by the Oficina de Asuntos para las Personas con Impedimentos (OAPI) of the Dean of Students. Likewise, students with special needs that require some type of accommodation must contact the professor.

## **Acomodo Razonable**

La Universidad de Puerto Rico cumple con todas las leyes federales, estatales y reglamentos concernientes a discriminaci3n, incluyendo "The American Dissabilities Act" (Ley ADA) y la Ley 51 del Estado Libre Asociado de Puerto Rico. Los estudiantes que reciban servicios de rehabilitaci3n vocacional deben comunicarse con el (la) profesor(a) al principio del semestre para planificar el acomodo razonable y equipo de apoyo necesario conforme a las recomendaciones de la Oficina de Asuntos para las Personas con Impedimento (OAPI) del Decanato de Estudiantes. Una solicitud de acomodo razonable no exime al estudiante de cumplir con los requisitos academicos del curso.

## **Academic Integrity**

La Universidad de Puerto Rico promueve los más altos estándares de Integridad académica y científica. El Artículo 6.2 del Reglamento General de estudiantes de la UPR (Certificación Núm. 13, 2009-2010, de la Junta de Síndicos) establece que “la deshonestidad académica incluye, pero no se limita a: acciones fraudulentas, la obtención de notas o grados académicos valiéndose de falsas o fraudulentas simulaciones, copiar total o parcialmente la labor académica de otra persona, plagiar total o parcialmente el trabajo de otra persona copiar total o parcialmente las respuestas de otra persona o las preguntas de un examen, haciendo o consiguiendo que otra tome en su nombre cualquier prueba o examen oral o escrito, así como la ayuda o facilitación para que otra persona incurra en la referida conducta”. Cualquiera de estas acciones estará sujeta a sanciones disciplinarias en conformidad con el procedimiento disciplinario establecido en el Reglamento general de Estudiantes de la UPR vigente.

### **Disciplinary Action in case of academic dishonesty**

Grade D will be given.

## **Hostigamiento**

La Universidad de Puerto Rico prohíbe el discrimen por razón de sexo y género en todas sus modalidades, incluyendo el hostigamiento sexual. Según la Política institucional contra el Hostigamiento Sexual en la Universidad de Puerto Rico, Certificación Núm. 130, 2014-2015 de la Junta de Gobierno, si un estudiante está siendo o fue afectado por conductas relacionadas a hostigamiento sexual, puede acudir ante la Oficina de la Procuraduría Estudiantil, el Decanato de Estudiantes o la Coordinadora de Cumplimiento con Título IX para orientación y/o presentar una queja