Course Syllabus

Course Title	Artificial Intelligence for Chemistry	**CRN** (Course Reference Number)	EE6310
Subtitle	-	**Credit hour** (Lecture hours – Lab hours – Credit hours)	3-0-3
Course Format	Lecture ■ Discussion ☐ Laboratory ☐ Practicum ☐ Blended ☐ Online ☐ (Add)_____		
Course Description	Machine learning is accelerating the pace of research in chemical science, enabling the rapid discovery of new materials and innovative characterization. In this course, students will learn the basics of deep learning, and will be exposed to some of the successful machine learning models in the chemical science field, the application of which extends to chemistry, catalysis, and materials science. The course materials are designed to be practical and friendly for engineers without a computer science background. This course implement flipped learning. The students will watch the lectures before the class, and the students will work on problem set and the problem set will be discussed together. The course also will also include working on project involving developing a neural network model.		

P1. Course Information

Instructor	Prof. Geun Ho Gu	**Office**	Smart Park D6-410
Office Hours	TBD	**Office Telephone**	061-330-9689
		E-mail	ggu@kentech.ac.kr
Discipline	Chemistry, AI	**Prerequisite**	Undergraduate level chemistry Undergraduate level linear algebra Undergraduate level differential equation
Target Audience	Graduate students with engineering back grounds		
Course Reading & Resources			
Required Materials	- Lecture notes are provided - Deep Learning from scratch by Saito Goki, O'Reilly		
Other Recommended Materials (optional)	- Andrew Ng's machine learning class lectures on Youtube (https://www.youtube.com/playlist?list=PLLssT5z_DsK-h9vYZkQkYNWcItqhlRJLN) - Andrew Ng's deep neural networks lectures on Youtube (https://www.youtube.com/playlist?list=PLpFsSf5Dm-pd5d3rjNtIXUHT-v7bdaEIe)		
Course Access	This is an offline course. Learning materials will be available online.		
Technical & Academic Support	If you need any technical/academic assistance at any time during the course, please contact your instructor and/or course TA - Instructor: Prof. Geun Ho Gu		

P2. Course Objectives

Course Learning Objectives	Through this course you will: - Learn basic python - Understand the basic algorithms of machine learning - Apply machine learning models to practical problems
Course Learning Activities	To meet the objectives, you will: - Watch lecture before the class - Work on problem set before the class, and come to class prepared to discuss - Develop a machine learning model for the topic of your choice - Give a professional presentation of the developed machine learning model

P3. Topic Outline/Schedule

Important note: Refer to the course calendar for specific dates and times. Activity and assignment details will be explained in detail within each week's corresponding learning module. If you have any questions, please contact your instructor.

Overview			
Wk1	**02/26**	**Offline Lecture** Digital chemistry. Mathematics review.	
	02/29	**Discussion** Python basics 1. Read Chapter 1 of S. Goki.	
Wk2	**03/04**	**Discussion** Python basics 2.	
	03/07	**Discussion** Python basics 3.	
Wk3	**03/11**	**Discussion** Python basics 4.	
	03/14	**Discussion** Python basics 5.	
Wk4	**03/18**	**Discussion** Perceptron 1. Read Chapter 2 of S. Goki.	
	03/21	**Discussion** Perceptron 2.	
Wk5	**03/25**	**Discussion** Perceptron 3.	
	03/28	**Discussion** Neural Network 1. Read Chapter 3 of S. Goki.	
Wk6	**04/01**	**Discussion** Neural Network 2.	
	04/02	**Discussion** Neural Network 3.	(04/04보강)
Wk7	**04/08**	**Discussion** Neural Network Training 1. Read Chapter 4 of S. Goki.	
	04/11	**Discussion** Neural Network Training 2.	
Wk8	**04/14**	**Project proposal due**	
	04/15	**1-on-1 meeting** Project proposal Discussion	
	04/16	**Discussion** Neural Network Training 3.	(04/18보강)
Wk9	**04/22**	**Discussion** Backpropagation 1. Read Chapter 5 of S. Goki.	
	04/23	**Discussion** Backpropagation 2.	(04/25보강)
Wk10	**04/29**	**Discussion** Backpropagation 3.	
	05/02	**Discussion** Learning Techniques 1. Read Chapter 6 of S. Goki.	
Wk11	**05/06**	**어린이날 대체 공휴일**	
	05/09	**Discussion** Learning Techniques 2.	
Wk12	**05/13**	**Discussion** Learning Techniques 3.	
	05/16	**Discussion** Convolutional Neural Network 1. Read Chapter 7 of S. Goki.	
Wk13	**05/20**	**Discussion** Convolutional Neural Network 2.	
	05/23	**Discussion** Convolutional Neural Network 3.	
	05/27	**Discussion** Graph Convolutional Neural Network 1.	

	05/30	**Discussion** Graph Convolutional Neural Network 2.	
Wk15	**06/03**	**Discussion** Graph Convolutional Neural Network 3.	
	06/06	**현충일 공휴일**	
Wk16	**06/10**	**Project presentation 1**	
	06/13	**Project presentation 2**	

P4. Grading Policy

Graded Course Activities

Activity	Percentage
Attendance (replaced as the problem set submission)	35
Participation	35
Class project proposal	10
Class project presentation	20
Total	**100%**