New Course Outline

College of Engineering, National Taiwan University

1. Course Summary

<table>
<tr><td>Department</td><td colspan="3">Materials Science and Engineering (材料系)</td><td colspan="2">Instructor</td><td colspan="3">Nguyen Tuan Hung (阮俊興)</td></tr>
<tr><td>Title of the Course</td><td colspan="7">(Chinese) 材料人工智慧與計算方法
(English) AI and Computational Methods for Materials</td><td>□Taught in Mandarin
■Taught in English</td></tr>
<tr><td>Code of the Course</td><td>527 U3350</td><td>Class</td><td></td><td>Course credits</td><td>3</td><td colspan="2">□Required
■Elective</td><td>□Full year
■Half year</td></tr>
<tr><td>Lecture Day/Time</td><td></td><td>Location</td><td></td><td>Maximum number of students</td><td>50</td><td colspan="2">Target students</td><td>□1st yr □2nd yr
■3rd yr ■4th yr</td></tr>
<tr><td>Website</td><td colspan="8"></td></tr>
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2. Syllabus (corresponding to CEIBA; English and Chinese)

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<tr><td>Course Description</td><td>This course will introduce modern computational methods for materials science, including artificial intelligence (AI), machine learning (ML) and density functional theory (DFT). Both AI/ML and DFT are becoming standard tools in chemistry, physics, and materials science. Deep learning specifically involves linking input data (features) with output data (labels) through a neural network. Neural networks are capable of approximating any function. A typical example is the relationship between a material's structure and its properties. Conversely, DFT is a computational method used to analyze the electronic structure of atoms, molecules, and materials. It is based on quantum mechanics and provides valuable insights into the properties and behavior of various materials. Both DFT and AI/ML have their own strengths and applications, and they can be combined. Depending on the engineering field and the specific problem, these methods can be relevant. Therefore, AI/ML and DFT are valuable tools for students who will become engineers and scientists.</td></tr>
<tr><td>Course Objectives/ Learning Goals</td><td>1) Understanding the DFT and AI/ML concepts.
2) Can practice the DFT and AI/ML by using the open-source Quantum ESPRESSO, TensorFlow, and Pytorch.
3) Using the dataset from the Material Project.
4) Apply DFT and AL/ML for practical applications in material science, such as screening solar cell materials.</td></tr>
<tr><td>Keywords</td><td>Artificial intelligence, Machine learning, Density functional theory, Quantum ESPRESSO, TensorFlow, and Pytorch, Material Project.</td></tr>
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Prerequisites (needed skills or required abilities in advance)	Know Linux and Python at basic level.
Mandatory Reading (Textbooks)	I. Goodfellow, Y. Bengio and A. Courville, Deep Learning, MIT Press, 800 Pages, (2016) N. T. Hung, A. R. T. Nugraha and R. Saito, Quantum ESPRESSO Course for Solid-State Physics, Jenny Stanford Publishing, New York, 372 Pages, (2022).
Other Recommended Literature	MIT Introduction to Deep Learning | 6.S191 https://www.youtube.com/playlist?list=PLtBw6njQRU-rwp5__7C0oIVt26ZgjG9NI Quantum ESPRESSO for Solid State Physics https://nguyen-group.github.io/courses/qe/
Grading (Percentages)	* Mid-semester examination (50%): 3 hours * Final examination (50%): 3 hours
Weekly Schedule	
Week	Topic
1	Introduce Python and install the computing environment.
2	Math review: Tensors and shapes
3	Introduction to machine learning (ML)
4	ML concepts: Regression, model assessment, classification, and kernel learning
5	Introduction to deep learning
6	Graph neural networks (GNN)
7	Equivariant neural networks
8	Mid-semester examination
9	Introduction to material science
10	Application of ML in the material science
11	Introduction to density functional density (DFT) and Quantum ESPRESSO (QE)
12	Practical DFT with QE: Basics parameters

13	Practical DFT with QE: Advanced topics
14	Practical DFT with QE: Input generator
15	Combine DFT and ML
16	Final examination