IIT Mandi
Proposal for a New Course

Course number : EP502
Course Name : Informatics for Materials Design
Credit Distribution : *2-0-2-3*
Intended for : BTech 4th Year, M.Sc. Physics, PhD Scholars, M.Tech
Prerequisite : None
Mutual Exclusion : None

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1. Preamble:

The rapid growth of computational technology and information science has led to a new era of advancement in materials science. In past decade, many materials databases have emerged where the theoretical as well as experimental data is collected. But it is not easy to use these databases without huge amount of pre-processing, data integration and deeper domain knowledge. Few efforts using the data-driven approach have shown that the machine learning models that enable rapid predictions based on the past data is a promising approach for material design. But the field of material design using informatics is still in infancy. The objective of this course is to introduce the students to the fast-growing field of material informatics.

Course Modules with quantitative lecture hours (2 Credits):

Unit/Topic 1: (4 Hours) Computational material science:
Crystal Structure and symmetry, Material properties, Property based classification of materials (mechanical, electrical, thermal, magnetic, optical), Performance of materials, Meta materials, Need for new materials.

Unit/Topic 2: (9 Hours) State of art techniques at different length scales
Concept of multiscale modeling, First principles approach, Density Functional Theory (electronic level), Brief introduction to Schrodinger's equation, Overview of most commonly used approximations (Born Oppenheimer, Local Density Approximations), Kohn-Sham equations, Pseudopotentials, Description of the self-consistent field iterations, Total energy minimization, Overview of major algorithms in DFT calculations.

Unit/Topic 3: (6 Hours) Databases and Python Scripting
DBMS fundamentals, Design, Workflows, Query writing, python libraries: Numpy, Panda, Pymatgen, Materials database repositories, Materials open database integration APIs.

Unit/Topic 4: (9 Hours) Introduction to Machine learning for material design
Philosophy behind machine learning, Basic vocabulary terms, Algorithms based on learning: supervised and unsupervised, Regression vs. classification, Regression algorithms, Clustering algorithms, Decision tree algorithms, Interpretability analysis using Lyme/Shap. Model independent Descriptors for material data analytics.

Laboratory/practical/tutorial Modules:

Lab work (1 Credit)

1. Hands on with Quantum Espresso (QE)- 3 Labs
2. Hands on with MySQL- 1 Lab
3. Working with python scripts, use of APIs etc – 2 Labs
4. Creating databases using APIs to fetch material data – 1 Lab
5. Machine learning with Scikit/Weka – 2 Labs

Research project (1 Credit): Based on use of machine learning/Quantum Espresso for understanding material design and its properties for particular applications like magnetic storage, photovoltaic response, electrical conductivity, magnetism and spintronic application.

2. Text books:*(Relevant and Latest, Only 2*)

1. ***June Gunn Lee, Computational Materials science, CRC press,USA 2012***
2. **Aurélien Géron, Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 2nd Edition, O'Reilly Media, Inc. 2019**

3. References:

- ***Online resources for learning SQL, python***
- ***Research papers***

4. Similarity with the existing courses:
(Similarity content is declared as per the number of lecture hours on similar topics)

S. No.		Course Code	Similarity Content	Approx. % of Content
1.		CS660, CS309, PH523, PH621	This course draws various modules from few courses as per the need of the interdisciplinary nature of the course.	None

6. Justification of new course proposal if cumulative similarity content is >30%: