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## Materials Genomics

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3    **Abstract**

4    This course introduces students to materials genomics, treating the periodic table and  
5    all known crystal structures as a searchable, computable design space. Students learn  
6    how materials databases are built, how to represent matter as numbers, graphs, or  
7    fingerprints, how to interrogate and predict properties of solids, how to use ML as a  
8    surrogate for quantum mechanics, and how to design new materials algorithmically.

9    **1 Course Information**

10    **4th Semester – 5 ECTS · 2h lecture + 2h exercises per week, together  
11    with ML for Materials Processing & Characterization**

12    **2 Course Philosophy**

13    Materials genomics treats the periodic table and all known crystal structures as a  
14    giant searchable, computable design space.

15    Students learn:

- 16    • how materials databases are built,
- 17    • how to represent matter as numbers, graphs, or fingerprints,
- 18    • how to interrogate and predict properties of solids,
- 19    • how to use ML as a surrogate for quantum mechanics,
- 20    • how to design new materials algorithmically.

21    **3 Week-by-Week Curriculum (14 weeks)**

22    **3.1 Unit I — Foundations of Materials Genomics (Weeks 1–3)**

23    **3.1.1 Week 1 – What is Materials Genomics?**

- 24    • Genomics analogy: genes → functions vs atoms → properties.
- 25    • Brief history: AFLOW, OQMD, Materials Project, NOMAD.
- 26    • PSPP from the structure-first viewpoint.

27    **Exercise:** Explore Materials Project; query bandgaps, energies, symmetries.

28    **3.1.2 Week 2 – Crystal structure fundamentals**

- 29    • Space groups, Wyckoff positions, symmetry operations.
- 30    • How symmetry informs descriptors.

31    **Exercise:** Using pymatgen / spglib to analyze symmetries.

32    **3.1.3 Week 3 – Materials databases & file formats**

- 33    • CIF, POSCAR, PDB-like formats.
- 34    • Thermodynamic quantities in databases: formation energy, stability, convex  
35    hull.

36    **Exercise:** Parse CIF files, extract primitive cells, compute density.

37    **3.2 Unit II — Representations of Materials (Weeks 4–6)**

38    **3.2.1 Week 4 – Classical descriptors & materials fingerprints**

- 39    • Magpie, matminer.
- 40    • Stoichiometric, elemental, and structural features.

41    **Exercise:** Build a small property regressor with Magpie features.

42    **3.2.2 Week 5 – Graph-based representations**

- 43    • Crystal structures as graphs: nodes, edges, periodic boundary conditions.
- 44    • CGCNN, MEGNet architecture intuition (no training from scratch yet).

45    **Exercise:** Build a simple CGCNN-like graph featurizer.

46    **3.2.3 Week 6 – Local atomic environments**

- 47    • Voronoi tessellations, coordination numbers, SOAP descriptors.

- 48       • Role in interatomic potentials and ML force fields.

49       **Exercise:** Compute SOAP vectors; perform clustering in descriptor space.

50       **3.3 Unit III — High-Throughput Computation & Screening (Weeks 7–9)**

51       **3.3.1 Week 7 – Quantum mechanical data and DFT basics**

- 52       • What DFT gives you: energies, forces, band structures, elastic constants.  
 53       • Why it's expensive; why ML surrogates matter.

54       **Exercise:** Run a toy DFT calculation (Quantum Espresso or MP workflows).

55       **3.3.2 Week 8 – High-throughput workflows**

- 56       • Automation: pymatgen, custodian, FireWorks, Atomate.  
 57       • Data generation for building surrogate models.

58       **Exercise:** Perform a small FireWorks workflow (or simulate the idea without cluster  
 59       resources).

60       **3.3.3 Week 9 – Phase stability & the convex hull**

- 61       • Formation energies, metastability, hull distance.  
 62       • Mapping an entire chemical system.

63       **Exercise:** Reconstruct phase diagrams from Materials Project data.

64       **3.4 Unit IV — Learning Properties from Atomic Structure (Weeks 10–12)**

65       **3.4.1 Week 10 – Regression on crystal data**

- 66       • Predicting bandgaps, hardness, elastic moduli.  
 67       • Comparing different representation families.

68       **Exercise:** Benchmark random forest, GPR, CGCNN on a small dataset.

69       **3.4.2 Week 11 – Machine-learned interatomic potentials**

- 70       • Overview: GAP, SNAP, MTP, NequIP.  
 71       • Role in simulating defects, diffusion, mechanical behavior.

72       **Exercise:** Fit a tiny ML potential (ACE or simple SNAP-style) to toy data.

73       **3.4.3 Week 12 – Generative models for materials**

- 74       • VAEs, diffusion models for crystal generation.  
 75       • Constraints: symmetry, stability, charge neutrality.

76       **Exercise:** Sample a generative model from a pretrained online source; analyze  
 77       validity.

78       **3.5 Unit V — Mini-Project & Synthesis (Weeks 13–14)**

79       **3.5.1 Week 13 – Project workshop**

80       **Example projects:**

- 81       • Predict bandgap from composition + structure representation.  
 82       • Identify new stable compounds in a chemical system.  
 83       • Build a graph-based model for elastic constants.  
 84       • Use ML to approximate formation energies for a ternary subsystem.  
 85       • Analyze SOAP fingerprints across polymorphs.

86       **3.5.2 Week 14 – Presentations & Reflection**

- 87       • Interpreting models: SHAP for materials descriptors.  
 88       • Strengths/limitations of materials genomics vs experiment-driven ML.  
 89       • How computational and experimental ML meet in modern labs.

90       **4 Learning Outcomes**

91       Students completing this course will be able to:

- 92     • Navigate major materials databases and extract relevant structural/property  
93        data.
- 94     • Represent crystals numerically using descriptors, fingerprints, and graphs.
- 95     • Train ML models to predict quantum-mechanical and thermodynamic proper-  
96        ties.
- 97     • Analyze structural features via symmetry, coordination, and environments.
- 98     • Perform high-throughput screening of materials candidates.
- 99     • Understand and apply generative models for inorganic crystals.
- 100    • Critically evaluate ML results in computational materials discovery.