AI in Material Science

Course Syllabus

Course Code: MSE 688
Credits: 3
Instructor: Dr. Burhan Beycan
Duration: 14 weeks
Prerequisites: Linear Algebra, Probability & Statistics, Materials Science Fundamentals, Programming Experience

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Course Description

This advanced course explores the intersection of artificial intelligence and materials science, focusing on machine learning applications for materials discovery, design, and optimization. Students will learn state-of-the-art AI techniques specifically tailored for materials research, including deep learning for crystal structure prediction, reinforcement learning for materials design, and generative models for novel materials discovery.

Learning Objectives

Upon completion of this course, students will be able to:

1. **Apply deep learning architectures** to materials science problems
2. **Implement graph neural networks** for crystal property prediction
3. **Design generative models** for novel materials discovery
4. **Utilize reinforcement learning** for materials optimization
5. **Develop computer vision techniques** for materials characterization
6. **Create end-to-end AI pipelines** for accelerated materials research

Course Outline

Week 1-2: Foundations of AI in Materials Science

- Overview of AI applications in materials research
- Materials representation for machine learning
- Feature engineering and descriptor development
- Introduction to materials informatics platforms

Week 3-4: Deep Learning Fundamentals

- Neural network architectures for materials
- Convolutional neural networks (CNNs)
- Recurrent neural networks (RNNs)
- Attention mechanisms and transformers

Week 5-6: Graph Neural Networks for Materials

- Graph representation of crystal structures
- Graph convolutional networks (GCNs)
- Crystal Graph Convolutional Neural Networks (CGCNN)
- Message passing neural networks

Week 7-8: Generative Models for Materials Discovery

- Variational autoencoders (VAEs) for materials
- Generative adversarial networks (GANs)
- Conditional generation of materials
- Latent space exploration and optimization

Week 9-10: Reinforcement Learning Applications

- Multi-armed bandits for materials screening

- Q-learning for synthesis optimization
- Policy gradient methods
- Active learning strategies

Week 11-12: Computer Vision for Materials Characterization

- Image analysis of microstructures
- Automated defect detection
- Phase identification from microscopy
- Real-time monitoring of synthesis processes

Week 13-14: Advanced Topics and Future Directions

- Physics-informed neural networks
- Uncertainty quantification in AI models
- Explainable AI for materials science
- Integration with experimental workflows

Assessment Methods

Component	Weight	Description
Programming Assignments	40%	Implementation of AI algorithms for materials
Research Project	35%	Novel AI application to materials problem
Literature Review	15%	Critical analysis of recent AI-materials papers
Presentation	10%	Project presentation and peer evaluation

Required Software and Frameworks

Deep Learning Frameworks

- **PyTorch** or **TensorFlow** for neural networks

- **PyTorch Geometric** for graph neural networks
- **DGL (Deep Graph Library)** for graph-based models

Materials Science Libraries

- **Pymatgen** for materials analysis
- **ASE** for atomic structure manipulation
- **CGCNN** implementation
- **MATMINER** for feature generation

Specialized Tools

- **OpenAI Gym** for reinforcement learning
- **RDKit** for molecular representations
- **SMACT** for materials composition analysis

Textbooks and Resources

Primary References

- **"Deep Learning"** by Ian Goodfellow, Yoshua Bengio, and Aaron Courville
- **"Hands-On Machine Learning"** by Aurélien Géron
- **"Graph Neural Networks: Foundations, Frontiers, and Applications"** by Lingfei Wu et al.

Research Papers and Reviews

- Recent publications in Nature Machine Intelligence
- Materials-focused papers from ICML, NeurIPS, ICLR
- Journal of Chemical Information and Modeling articles

Laboratory Projects

Project 1: Crystal Property Prediction with GNNs

Implement and train graph neural networks to predict formation energies and band gaps of crystalline materials using the Materials Project database.

Project 2: Generative Materials Design

Develop a variational autoencoder to generate novel crystal structures with desired properties, focusing on specific material classes (e.g., perovskites, Heusler alloys).

Project 3: Reinforcement Learning for Synthesis Optimization

Create a reinforcement learning agent to optimize synthesis parameters for achieving target material properties in a simulated environment.

Project 4: Computer Vision for Microstructure Analysis

Build a convolutional neural network to automatically classify and quantify microstructural features from scanning electron microscopy images.

Advanced Topics Modules

Module A: Physics-Informed Neural Networks (PINNs)

- Incorporating physical laws into neural network training
- Applications to phase field modeling
- Solving partial differential equations for materials

Module B: Federated Learning for Materials

- Collaborative learning across institutions
- Privacy-preserving materials research
- Distributed model training strategies

Module C: Quantum Machine Learning

- Quantum algorithms for materials simulation
- Variational quantum eigensolvers
- Quantum-classical hybrid approaches

Industry and Research Connections

Guest Speakers

- AI researchers from Google DeepMind, Microsoft Research
- Materials scientists from national laboratories
- Industry practitioners from materials companies

Collaborative Projects

- Partnership with experimental research groups
- Integration with high-throughput synthesis facilities
- Connection to materials genome initiative projects

Grading Scale

Grade	Percentage	Description
A	90-100%	Outstanding innovation and technical excellence
B	80-89%	Strong performance with good technical depth
C	70-79%	Satisfactory work meeting basic requirements
D	60-69%	Below average with significant weaknesses
F	<60%	Unsatisfactory performance

Course Policies

Computational Resources

Access to GPU clusters for training deep learning models. Students may also use cloud computing credits for large-scale experiments.

Reproducibility Requirements

All code must be version-controlled and documented. Experiments should be reproducible with provided random seeds and environment specifications.

Ethical AI Considerations

Discussion of bias, fairness, and responsible AI practices in materials research. Consideration of environmental impact of large-scale AI computations.

Open Science Practices

Encouragement to share code, data, and models through appropriate repositories. Discussion of intellectual property considerations in collaborative research.

Final Project Options

Option 1: Novel Algorithm Development

Develop a new AI algorithm specifically designed for a materials science application, with theoretical justification and empirical validation.

Option 2: Comprehensive Application Study

Apply multiple AI techniques to solve a complex materials challenge, comparing approaches and providing insights for the materials community.

Option 3: Integration with Experimental Workflows

Design and implement an AI system that integrates with experimental equipment for real-time decision making in materials synthesis or characterization.

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