AI and Materials 4/12

Schedule

8.30 Coffee + sandwich

9.00 Welcome by Martin Ek

9.15 **Rickard Armiento** (Linköping University): AI/ML in materials science: Screening the unexplored crystal prototype space

10.00 **Alena Vishina** (Uppsala University): Data-driven design of high-performance permanent magnets

10.45 Break

11.00 NanoLund presenters

Mattias Borg (Electrical and Information Technology): Analog computing in memory – towards sustainable AI

Knut Deppert (Physics): Nanoparticles (TBD)

Vanya Darakchieva (Physics): Semiconductor materials (TBD)

Maning Liu (Chemistry): Halide Perovskite and Perovskite-Inspired Nanomaterials for Diverse Light Energy-Converting Applications

Filip Lenrick (Mechanical Engineering Sciences): Metal processing by chemical vapors

12.15 Lunch

13.00 **Kristian Thygesen** (Technical University of Denmark): Data-driven material design of thin film and 2D semiconductors

13.45 **Tomas Olsson** (RISE Swedish Institute of Computer Science): Introduction to Large Language Models and their impact to scientific discovery in materials design

14.20 Coffee and discussion with presenters

15.00 Concluding remarks by Vanya Darakchieva

15.15 End

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Support by: Nanoscience and Semiconductor Technology Profile Area, AI Lund

Speaker: Rickard Armiento (LiU)
Title: AI/ML in materials science: Screening the unexplored crystal prototype space
This talk covers the application of AI/ML methods in materials science and design. An overview of a few selected methods and related topics is given. One key area is the creation and curation of training data, emphasizing the importance of data standardization efforts like OPTIMADE [1]. I will discuss the merits of fine-grained vs. coarse-grained descriptors. In particular, I will talk about the WREN (Wyckoff REpresentation regressioN) model trained to predict properties for element-assigned crystal prototypes expressed via Wyckoff positions [2].

This model allows screening for materials with desired properties with structures fundamentally different from those already present in materials databases. The ability to screen for new materials is demonstrated by resolving XRD patterns. Our highly efficient GPU-accelerated implementation allows systematic enumeration of the chemi-structural space of candidate prototypes, ordering them by predicted formation energy, and optimizing all degrees of freedom to match the XRD peaks. The approach is shown to resolve previously unresolved XRD patterns in the ICDD database to uncover completely new crystal structures, i.e., with prototypes not present in current materials databases [3].

[1] https://www.nature.com/articles/s41597-021-00974-z
[2] https://www.science.org/doi/10.1126/sciadv.abn4117
[3] https://doi.org/10.48550/arXiv.2106.11132

Speaker: Alena Vishina (UU)
Title: Data-driven design of high-performance permanent magnets
High-performance permanent magnets (PMs) are an essential part of an electric motor and are in high demand for green energy transition. Each wind turbine contains up to 400 kg of magnetic materials, while an electric car carries about 2 kg. At the same time, all high-performance magnets currently in use contain rare-earth elements, which is undesirable for several economic and environmental reasons. Hence, there is a growing interest in finding rare-earth-free or rare-earth-lean alternatives with similar prize performance.

Unlike the common approach to the problem where researchers look into a promising crystal structure or combination of elements, we use a high-throughput technique to look for the desired properties among the materials of several databases. The criteria of a promising candidate material are high magnetization, uniaxial magnetocrystalline anisotropy, high Curie temperature, and more. When an interesting material is found by filtering through the entries of a database, we investigate the ways to improve its qualities by element substitution or doping.

Speaker: Kristian Thygesen (DTU)
Title: Data-driven material design of thin film and 2D semiconductors
Automated workflows for data generation and -exploitation (supervised and unsupervised) have long been employed in fields like bio-chemistry and drug discovery, but are only now making their way into materials science. I will begin this talk by introducing the Atomic Simulation Recipes (ASR) – an open source Python framework for constructing and executing materials simulation workflows[1,2]. Next, I will give some examples of its use in materials design studies including the search for indirect band gap semiconductors for thin-film photovoltaics [3] and the Computational 2D Materials Database (C2DB), which contains calculated properties of several thousand 2D materials in monolayer and bilayer form [4]. Finally, I will discuss how deep generative models can help to suggest new types of materials by learning the patterns in known data sets of stable materials [5]. If time allows, I will discuss machine learning of GW band structures from descriptors encoding the electronic structure of standard DFT calculations.[6]

[1] MyQueue: Task and workflow scheduling system, Mortensen *et al.*, 2020 *Journal of Open Source Software, 5(45), 1844, https://doi.org/10.21105/joss.01844*
[2] The atomic simulation environment—a Python library for working with atoms, Larsen *et al.*, 2017 *J. Phys.: Condens. Matter*, 29, 273002,https://doi.org/10.1088/1361-648X/aa680e

[3] Indirect Band Gap Semiconductors for Thin-Film Photovoltaics: High-Throughput Calculation of Phonon-Assisted Absorption, J. *Am. Chem. Soc.* 2022, 144, 43, 19872–19883, https://doi.org/10.1021/jacs.2c07567
[4] Recent progress of the Computational 2D Materials Database (C2DB), Morten Niklas Gjerding *et al* 2021 *2D Mater.* 8 044002, DOI: 10.1088/2053-1583/ac1059
[5] Data-driven discovery of 2D materials by deep generative models, P. Lyngby and K. Thygesen, *npj Computational Materials* **8**, 232 (2022)
[6] Representing individual electronic states for machine learning GW band structures of 2D materials, N. Knoesgaard and K. Thygesen, *Nature Communications* **13**, 468 (2022)