Ihor Neporozhnii

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Education

University of Toronto **Sep. 2021 – Present**
PhD – Physical and Environmental Sciences *Toronto, Canada*
Developing computational tools to accelerate the discovery of materials for clean energy applications.

Taras Shevchenko National University of Kyiv **Sep. 2017 – Jun. 2021**
Bachelor of Science – Physics and Astronomy *Kyiv, Ukraine*
Specialized in computational Nuclear and High-energy Physics

Technical Skills

Programming Languages: Python (numpy, pandas, scipy, matplotlib), R, Julia, C++
Machine Learning: PyTorch, TensorFlow, XGBoost, Scikit-learn, Flux ML
High-performance computing: remote calculations on GPU and CPU clusters
Computational Chemistry: VASP, CP2K, DFTB+
High-energy Physics: CERN Root, Geant 4
Version control (Git, GitHub), Docker, Linux, MacOs

Research and Work Experience

University of Toronto, Clean Energy Lab **September 2021 – Present**
Research Assistant, Supervisor: Prof. Oleksandr Voznyy *Toronto, Canada*

- I develop and apply computational tools to accelerate the discovery of materials. In the course of my research, I have been extensively using programming languages **(Python, R, Julia)**, machine learning libraries **(PyTorch, Tensorflow, XGBoost, Scikit-learn)**, and Density Functional Theory codes **(VASP, CP2K, DFTB+)**. I developed a Graph Neural Network that reduced the computational cost of electronic structure predictions by $\times\mathbf{10,000}$ times.
- In my research I use **GPU** and **CPU clusters** of the Digital Research Alliance of Canada to train Machine Learning models and conduct Quantum Chemistry calculations.

Alliance For AI-Accelerated Materials Discovery (A3MD) at UofT **April 2023 – Present**
BootCamp Facilitator and Instructor *Toronto, Canada*

- I facilitate 5-day BootCamps on **Machine Learning** for Research Scientists at **LG** and **Total Energies**.

University of Toronto **September 2021 – Present**
Practice Leader *Toronto, Canada*

- I conduct practical sessions for students enrolled in courses Physics I and Physics II.

University of Toronto **June 2020 – August 2021**
Research Intern *Toronto, Canada*

- Developed **Neural Networks** with **PyTorch** to predict properties of materials.

CNRS, Université Paris-Saclay **March 2021 – April 2021**
Research Intern *Paris, France*

- Developed an algorithm to analyze signals from JUNO neutrino experiment. Implemented the algorithm in **C++** which resulted in a **50%** improvement in the accuracy of signal reconstruction.

Institute of Physics, National Academy of Sciences of Ukraine **April 2019 – August 2021**
Engineer *Kyiv, Ukraine*

- Conducted experiments with nanomaterials in ultra-high vacuum conditions.

Jagiellonian University **July – August 2020**
Research Intern *Krakow, Poland*

- Performed cross-match of neutrino and Gamma-ray burst datasets, conducted statistical analysis with **Python**.

Institute of Nuclear Physics, Polish Academy of Sciences **July – August 2019**
Research Intern *Krakow, Poland*

- Analyzed data from CERN Atlas experiment using **Machine Learning** and **Monte Carlo** methods.

Publications

Navigating Materials Space with ML-Generated Electronic Fingerprints **2023**
I. Neporozhnii, *Z. Wang, R. Bajpai, C. Gomez, N. Chakraborty, I. Tamblyn, O. Voznyy* *Preprint*
doi: https://doi.org/10.26434/chemrxiv-2023-j1szt

I developed a Graph Neural Network (GNN) for the prediction of materials Density of States and used it to create a space with **150,000** *chemical compounds structured by the similarity of their properties. The GNN reduced the computational cost from* **$5.0** *to* **$0.0005** *per material allowing us to scale the approach to much larger material spaces.*

Strain data augmentation enables machine learning of inorganic crystal geometry optimization **2023**
F. Dinic, Z. Wang, **I. Neporozhnii**, *U. Bin Salim, R. Bajpai, N. Rajiv, V. Chavda,* *Patterns*
V. Radhakrishnan, and O. Voznyy. doi: https://doi.org/10.1016/j.patter.2022.100663

I developed a machine learning (ML) model that enables accurate prediction of the formation energy for non-equilibrium structures which previously required computationally expensive DFT calculations.

Insertion of MXene-Based Materials into Cu–Pd 3D Aerogels for Electroreduction of CO2 to Formate **2023**
Advanced Energy Materials
M. Abdinejad, S. Subramanian, M. K. Motlagh, M. Noroozifar, S. Duangdangchote,
I. Neporozhnii, *D. Ripepi, D. Pinto, M. Li, K. Tang, J. Middelkoop, A, Urakawa,*
O. Voznyy, H.-B. Kraatz, T. Burdyny. doi: https://doi.org/10.1002/aenm.202300402

I conducted Density Functional Theory (DFT) calculations using VASP software.

Mesoscopic self-ordering in oxygen doped Ce films adsorbed on Mo(112) **2021**
T. Afanasieva, A. Fedorus, A. Goriachko, A. Naumovets, **I. Neporozhnii**, *and D. Rumiantsev.* *Surface Science*
doi: https://doi.org/10.1016/j.patter.2022.100663

I conducted experiments with nanomaterials in ultra-high vacuum conditions.

Conference Presentations

Accelerate Conference 2023 (Poster, presenter) **August 2023**
Acceleration Consortium, University of Toronto *Toronto, Canada*

Climate Positive Energy Research Day (Talk, invited speaker) **August 2023**
University of Toronto *Toronto, Canada*

CSC 2023 (Talk, presenter, received presentation award) **June 2023**
The Chemical Institute of Canada *Vancouver, Canada*

MRS Fall Meeting & Exhibit 2022 (Talk, presenter) **December 2022**
Material Research Society *Boston, United States*

Accelerate Conference 2022 (Poster, presenter) **August 2022**
Acceleration Consortium, University of Toronto *Toronto, Canada*

CSTCC 2022 (Poster, presenter) **June 2022**
Canadian Association of Theoretical Chemists *Kelowna, Canada*

CCCE 2022 (Talk, presenter) **June 2022**
The Chemical Institute of Canada *Calgary, Canada*

WDS 2020 (Talk, presenter)) **September 2020**
Charles University *Prague, Czech Republic*

Scholarships and Awards

Climate Positive Energy Graduate Student Scholarship **2023 – 2024**
University of Toronto, Climate Positive Energy *Total value: $15,000*

Connaught International Scholarship for Doctoral Students **2021 – 2024**
University of Toronto *Total value: $30,000*

Certificates

- Data Science certificate (University of Toronto, SciNet)
- Neural Networks and Deep Learning by Coursera (Deeplearning.ai)