MARIYA POPOVA

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EDUCATION

University of North Carolina at Chapel Hill **Expected May 2022**
PhD, Bioinformatics and Computational Biology
- Selected coursework: Structural Bioinformatics, Sequence Modelling, Mathematical Modelling

Moscow Institute of Physics and Technology, Moscow, Russia **July 2017**
Master of Science, Applied Mathematics and Physics (double degree program)
- Thesis project: Generative and Predictive models for producing novel molecular compounds
- Selected coursework: Image Processing and Recognition, Signals and Multidimensional Data Processing, Regression Analysis

Skolkovo Institute of Science and Technology, Moscow, Russia **June 2017**
Master of Science, Mathematics and Computer Science (double degree program)
- Thesis project: Deep Reinforcement Learning for de-novo drug design
- Academic excellence award
- Selected coursework: Numeric Linear Algebra, Optimization Methods, Machine Learning, Deep Learning, Bayesian Methods – Advanced Machine Learning, Probabilistic Graphical Models

Moscow Institute of Physics and Technology, Moscow, Russia
Bachelor of Science, Applied Mathematics and Physics **July 2015**
- Thesis project: Selection of an optimal neural network model for multi-class time series classification

SKILLS

Programming/Scripting Languages: Python, Java, Matlab, R
Frameworks and Tools: PyTorch, Theano, Lasagne, PyMol, PyRosetta

EXPERIENCE

Deep Learning Software Engineer Intern **Summer 2018**
NVIDIA Corporation
- Developed an open-source Deep Learning toolkit for Computational Chemistry and Drug Design

Visiting Research Scholar
University of North Carolina at Chapel Hill **Oct 2016 – Mar 2017**
- Developed a Deep Learning model (Python + Lasagne) for computational design of chemical compounds with optimized properties
- Patent application submitted

Research Intern **June 2016 – August 2016**
Yandex LLC CERN Research Group, Moscow, Russia
- Developed a Reinforcement Learning prototype (Python + Lasagne) for treatment optimization of patients with liver disease

SELECTED PROJECTS

OpenChem: Deep Learning toolkit for Computational Chemistry and Drug Design
NVIDIA Corporation, University of North Carolina at Chapel Hill
- Toolkit for Computational Chemistry with PyTorch backend aimed to make Deep Learning models an easy-to-use tool for Computational Chemistry and Drug Design Researchers
- Available at https://github.com/Mariewelt/OpenChem

De Novo Drug Design with Deep Reinforcement Learning
University of North Carolina at Chapel Hill
- Deep learning library with Pytorch backend for generation of ligands with target-biased properties
- Available at https://github.com/isayev/ReLeaSE

HONORS AND AWARDS

NVIDIA Graduate Fellow **2019/2020 academic year**
- The fellowship program supports graduate students doing GPU-based work

Molecular Sciences Software Institute (MolSSI) Seed Software Fellowship **2019**
- Awarded to graduate students and postdocs pursuing the development of software infrastructure, middleware, and frameworks that will benefit the broader field of computational molecular sciences

SELECTED PUBLICATIONS

1. **M. Popova**, O. Isayev, A. Tropsha, Deep reinforcement learning for de novo drug design. *Science Advances.* 4 (2018), doi:10.1126/sciadv.aap7885.