

Chapter 2

MACHINE LEARNING

Keynote Abstract: 2, Introducing Keynote Speaker Mr. Bogdan Penkovsky

Towards autonomous API synthesis with deep reinforcement learning

Reinforcement learning (RL) is a general learning and decision making paradigm based on interaction with the environment. Despite being challenging in practice, implementing RL for real world tasks could improve the safety and efficiency of autonomous processes. In this work we apply RL for an autonomous molecule synthesis with continuous flow chemistry. In our preliminary experiments, we demonstrate that our agent trained by deep reinforcement learning is capable of responding to real-time challenges, such as changes in the environment, sensor noise, and perturbations in order to ensure the optimal chemical synthesis conditions. The ultimate goal of this work is to conceive an autonomous chemical production unit for active pharmaceutical ingredients (API).

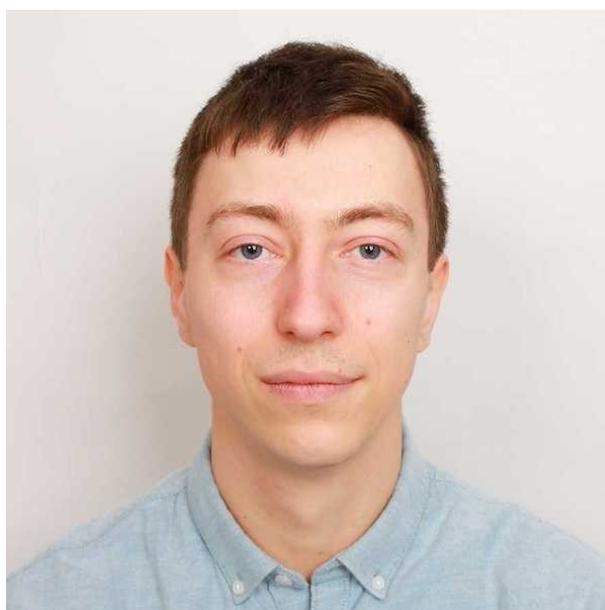


Figure 2.1: Mr. Bogdan Penkovsky (Alysophil SAS)