# Advanced Deep Learning Course for Chemistry

**Title**: Application of deep learning and reinforcement learning for molecule generation.

**Duration**: 12 hours of class work + independent work (~10 hours).

**Prerequisites**:
– Good command of Python.
– Computers equiped with GPU or Google Colab.
– Knowledge of deep learning basics (a good understanding of backpropagation is essential).

**Practical project**: Molecule generation through reinforcement learning.

**Summary**:
This course primarily focuses on reinforcement learning, a machine learning technique in which an agent learns to develop strategies for sequential actions. Participants will gain insights into the advantages and limitations of deep learning and deep reinforcement learning, explore various molecular representations, generate molecules, and visualize the outcomes.

Reinforcement learning emulates the learning processes observed in animals and humans, as studied in behavioral psychology. An RL algorithm learns by trial and error. Consequently, the agent is trained to maximize cumulative rewards. While reinforcement learning algorithms are highly powerful, users must develop specialized skills to utilize them properly.

**Macro-skills**:
- Understand and explain the benefits and limitations of deep learning.
- Know the very details of optimisation techniques such as adaptive moment estimation.
- Know the advantages and limitations of the different molecular representations.
- Visualize results for interpretation.
- Understanding reinforcement learning.
- Generating new molecules with desired properties.

**Instructor**: Bogdan Penkovsky (Alysophil).

**Course Evaluation**: Mini-project in groups of 2 or 3.

**Schedule** :
1. Advantages and limitations of deep learning [1-2].
2. Presentation of common tools such as adaptive moment estimation (Adam), convolutional neural networks, useful inductive biases, etc.
3. Generative models. Generation of molecules. Interpolation between molecules in the latent space.

4. Review: molecular representations used in Machine Learning and molecule generation.
5. Introduction to reinforcement learning [3-4,7].
6. Practice: Introduction to reinforcement learning [4]. Introduction to automated software validation.
7. Practice: Molecule generation with deep reinforcement learning [5].


[1] https://www.mdpi.com/2073-431X/12/5/91
[2] https://journalofbigdata.springeropen.com/articles/10.1186/s40537-021-00444-8
[3] https://penkovsky.com/neural-networks/beyond/
[4] https://github.com/huggingface/deep-rl-class
[5] https://chemrxiv.org/engage/chemrxiv/article-details/65463cafc573f893f1cae33a
[6] https://www.deeplearningbook.org
[7] http://incompleteideas.net/book/the-book-2nd.html