Jim Boelrijk | CV

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Education

2020-Now **PhD AI4Science**, *Amsterdam Machine Learning Lab (AMLAB), Universiteit van Amsterdam*, Amsterdam, The Netherlands
- Supervisors: Bernd Ensing, Patrick Forré, Bob Pirok and Alfons Hoekstra
- Topic of my PhD thesis:
  - Development of closed-loop optimization schemes using machine learning techniques.
  - Development of data-analysis techniques (peak detection, baseline correction, quantitative structure activity relationships) using machine learning techniques.

2017-2019 **Master Chemistry (Track: Molecular Sciences, GPA: 8.5/10, cum laude)**, *Universiteit van Amsterdam*, Amsterdam, The Netherlands
- Title of my master's thesis:
  Incorporating maximally localized Wannier functions into neural network potentials

2015-2017 **Bachelor Chemistry**, *Universiteit van Amsterdam*, Amsterdam, The Netherlands

2012-2013
- Title of my bachelor's thesis:
  Vibrational Circular Dichroism of Glucose: Dynamic vs Static approaches

2006-2012 **Bilingual VWO, profile: Nature and Technology with extracurricular Economics**, *Hermann Wesselink college*, Amstelveen, The Netherlands

Work Experience

2019-2020 **Software Tester**, *Software for Chemistry and Materials*, Netherlands
- Testing software changes in the AMS packages.
- Testing software of competition from installment to benchmarks.
- Creating general benchmark workflow in Python.

2013-2019 **Exam trainer**, *Lyceo*, Netherlands
- Preparing students for their high school exams in physics and chemistry.
- Learned to explain things clearly.

2016-2016 **Temporary teacher**, *Inwijs*, Netherlands
- Temporarily replaced a chemistry and physics teacher. Taught chemistry and physics to 5th- and 6th-year VWO high school students.
- Learned what it was like to plan lectures, explain matter to students and keep order.

2013-2015 **Professional Rugby Player**, *Stade Montois Rugby*, Mont-de-Marsan, France
- Was part of the youth academy (Under 23) of the professional rugby club Stade Montois.
- Learned to work hard, be disciplined and to not give up easily.
- Learned to adapt to a new environment and to the French language quickly.

Selected Publications

- **Boelrijk, J.**, Pirok, B., Ensing, B., and Forré, P. Bayesian optimization of comprehensive two-dimensional liquid chromatography separations. *Journal of Chromatography A*, 2021
- **Boelrijk, J.**, van Herwerden D., Ensing B., Forré P, and Samanipour S. Predicting RP-LC retention indices of structurally unknown chemicals from mass spectrometry data. *ChemRxiv.*, 2022, submitted to Journal of Cheminformatics
- Bos, T, **Boelrijk, J.**, Molenaar, S, van 't Veer, B, Niezen, L, van Herwerden, D, Samanipour, S, Stoll, Dwight, Ensing B., Forré P, Somsen, G and B. Pirok. Chemometric Strategies for Fully Automated Interpretive Method Development in Liquid Chromatography *ChemRxiv.*, 2022, submitted to Analytical Chemistry
- **Boelrijk, J.**, Ensing B., Forré P, and B. Pirok. Closed-loop automatic gradient design for liquid chromatography using Bayesian optimization. *ChemRxiv.*, 2022, submitted to Analytica Chimica Acta, 2022
- **Boelrijk, J.**, Ensing B. and Forré P. Multi-objective optimization via equivariant deep hypervolume approximation. *Arxiv.*, 2022, submitted to ML conference

Relevant Courses

Ab Initio Molecular Dynamics *MSc Chemistry, 8.0/10*

- Learned basic theoretical background and simple applications of Density Functional Theory based Molecular Dynamics (CP2K).

Applied Theoretical Chemistry *MSc Chemistry, 8.0/10*

- Learned to understand and predict molecular structure and chemical reactivity using ADF.

Biomolecular Simulations *MSc Chemistry, 8.5/10*

- Used Molecular Dynamics (GROMACS) to investigate the structure and dynamics of polyglutamine.

Quantum Theory of Molecules and Matter *MSc Chemistry, 7.5/10*

- Obtained basic quantum mechanics knowledge and its application to atoms, molecules and spectroscopy.

Understanding Molecular Simulation *MSc Chemistry, 8.0/10*

- Learned to understand and apply molecular simulations (In CPMD) and obtained insight in the underlying theory.

Numerical Techniques *MSc Chemistry, 8.0/10*

- Translated physical-chemical phenomena into mathematical models using sets of (non)linear equations and differential equations in MATLAB.

Relevant Skills

Programming

- Python
- Pytorch (including GPytorch and Botorch)
- Bash
- Matlab (limited)
- C++ (limited)

Language proficiency

- Dutch (native)
- English (bilingual)
- French (professional)
- German (limited working)

Awards and Achievements

- Youth player of the year 2012, best under 18 rugby player of the Netherlands
- Player for the National rugby team of the Netherlands (15 appearances so far).
- DELF B2 certificate in French.

Miscellaneous

Invited Talks

- AI4Science kickoff-workshop at the University of Amsterdam (09-07-2020)
- Illustere Alumni Event 2020 at the University of Amsterdam (19-11-2020)
- CHAINS KNCV Focus session on Machine learning for chemical discovery (07-12-2021)
- AMLAB Seminar at the University of Amsterdam (multiple)

Teaching

- Teaching Assistant for Deep Learning 1 2021 (Master AI, University of Amsterdam)
- Teaching Assistant for Machine Learning 2 2020-2021 (Master AI, University of Amsterdam)
- Teaching Assistant for Machine Learning 1 2020 (Master AI, University of Amsterdam)
- Teaching Assistant for MolSim 2021 (Master Molecular Sciences / 2 week PhD Winter course)

Organization

- Chair of the bi-weekly AI4Science Colloquium
- Maintenance of the AI4Science website

Summer Schools

- Deep Learning + Reinforcement learning Summer School 2021 (DLRLSS 2021)