

Jim Boelrijk CV

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in jim-boelrijk

Education

2020-Now **PhD Al4Science**, Amsterdam Machine Learning Lab (AMLAB), Universiteit van Amsterdam, Amsterdam, The Netherlands

- O 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 5thand 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

Relevant Skills

Programming

- Pvthon
- 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 (7 appearances so far).
- DELF B2 certificate in French.

Miscellaneous

Invited Talks

- Al4Science kickoff-workshop at the University of Amsterdam (09-07-2020)
- Illustere Alumni Event 2020 (19-11-2020)
- CHAINS KNCV Focus session on Machine learning for chemical discovery (07-12-2021)
- AMLAB Seminar (multiple)

Teaching

- Teaching Assistant for Deep Learning 1 2021 (Master AI, University of Amsterdam)
- Teaching Assistant for Machine Learning 2 20202021 (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 Al4Science Colloquium
- Maintenance of the AI4Science website