

**Institute for Materials Science** 

## **Dr. Alexander Wiltschko**

Google Brain

## "Learning to Smell: Using Deep Learning to Predict the Olfactory Properties of Molecules"

Thursday, June 10<sup>th</sup> 2021 16:00 – 17:00

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL) Pandemic version: https://tinyurl.com/nanoSeminar-GA

Predicting the relationship between a molecule's structure and its odor remains a difficult, decades-old task. This problem, termed quantitative structure-odor relationship (QSOR) modeling, is an important challenge in chemistry, impacting human nutrition, manufacture of synthetic fragrance, the environment, and sensory neuroscience. We propose the use of graph neural networks for QSOR, and show they significantly out-perform prior methods on a novel data set labeled by olfactory experts. Additional analysis shows that the learned embeddings from graph neural networks capture a meaningful odor space representation of the underlying relationship between structure and odor, as demonstrated by strong performance on two challenging transfer-learning tasks. Machine learning has already had a large impact on the senses of sight and sound. Based on these early results with graph neural networks for molecular properties, we hope machine learning can eventually do for olfaction what it has already done for vision and hearing.









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Alex Wiltschko is a staff research scientist at Google Brain, focusing on building more flexible machine learning software systems, and also applications of machine learning to biology. He has helped build several machine learning libraries at Twitter and Google, and also led research teams applying machine learning to basic scientific problems, and now works on chemistry and olfaction. He completed his PhD in Neurobiology at Harvard with Prof Sandeep Datta, studying the neuroscience of behavior and olfaction. He now leads a research team at Google Brain focusing on Al and machine learning for the sense of smell.





