

PHYSICAL CHEMISTRY SEMINAR



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Google Brain

Monday, Nov. 16, 2020

4:00 PM

via Zoom

“Machine learning for scent”



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 cutting-edge machine learning methods 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 separate tasks. Machine learning has already had a large impact on the senses of sight and sound. Based on these early results with neural networks for predicting molecular properties, we hope machine learning can eventually do for olfaction what it has already done for vision and hearing.