Molecular Translation: The Application of Deep Learning Language Models in Chemical Reaction Prediction

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It is common for experts in a field to draw linguistic analogies to their chosen discipline. People may refer to the Language of Mathematics or Physics for example. But for Chemists this analogy may be more real then not. Chemicals can have many representations, both visual and textual. Text-based representations of chemicals can allow for the application of multiple natural-langauge processing techniques to be applied to them. In this presentation I will be demonstrating how Deep Learning architectures for language translation can be reappropriated to the problem of predicting the outcome of chemical reactions. This talk will include discussion of chemical representations, the discussion of language translation models, and the comparisons of different model performances on a reaction prediction problem.

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