

Shocklab x Nitschke Lab Seminar #2

Molecule Design Based on
Multi-objective Optimisation
and Graph Transformers



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SAVE THE DATE

7 JUNE 2023

4 pm - 5 pm

Venue: UCT CS Building, CS203

Online link to be shared



ABSTRACT

In this talk I will present an empirical exploration of using machine learning and evolutionary algorithms to automate chemical product design. Our study demonstrates how computational design can be controlled via hyper-parameters to generate solutions with desired features and has important implications for automating chemical product design.

For more information

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