



Showcasing research from Professor Alexandre Tkatchenko's group, Department of Physics and Materials Science, University of Luxembourg, Luxembourg City, Luxembourg.

"Freedom of design" in chemical compound space: towards rational *in silico* design of molecules with targeted quantum-mechanical properties

This work demonstrates that "freedom of design" is a fundamental and emergent property of chemical compound space – the unfathomably vast space populated by all possible atomic compositions and their geometries. Such intrinsic flexibility enables rational design of distinct molecules sharing an array of targeted quantum-mechanical properties. The combination of the insights gained from this work with advanced machine learning approaches could aid in the development of effective strategies for high-throughput screening of novel molecules tailored to a specific application. Galaxy background image by pikisuperstar via Freepik.

As featured in:



See Leonardo Medrano Sandonas, Robert A. DiStasio, Jr, Alexandre Tkatchenko *et al.*, *Chem. Sci.*, 2023, 14, 10702.