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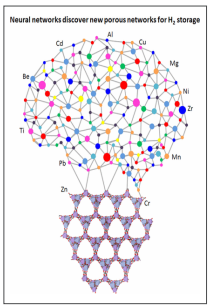
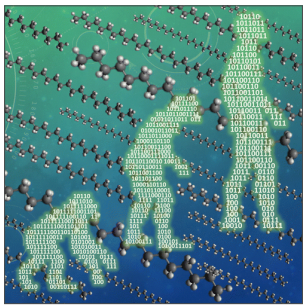
Discovering new green materials using AI and adaptive evolution





Materials research is expanding on many fronts, leveraging exciting developments in high throughput robotic synthesis and testing new mathematical methods, efficient algorithms and data handling and artificial intelligence and machine learning. These experiments provide large data sets that are ideal for generating data-driven computational models that can make quantitative predictions of properties of materials not yet synthesized. This allows large virtual libraries of materials to be rapidly screened computationally for promising candidates. It is now widely recognized that the number of materials that could be synthesized by chemistry is extremely large, essentially infinite. These vast materials spaces may be sparsely populated by islands of useful green materials so considerable effort is being applied to exploring them as efficiently as possible. An emerging paradigm for discovery of novel functional, yet safe and environmentally benign, materials involves the synergistic combination of high throughput experimentation, robust machine learning and feature selection algorithms and evolutionary processes. Most scientific innovations and technologies pass through the well-known S curve with slow beginning, an almost exponential growth in capability and a stable applications period. Adaptive, evolving, learning molecular design and optimization methods are approaching a period of very rapid growth and their impact is already being described as potentially disruptive. Ultimately, it may be possible to close the loop and generate autonomous materials discovery methods using these adaptive evolutionary methods and new mathematical techniques that can work back from model predictions to new materials. Effective exploitation of these potentially paradigm-shifting methods should result in a step change in the number and effectiveness of novel green molecules and materials available for broad applications in medicine and industry. I illustrate these methods and their application to design of safe-by-design nanomaterials, porous materials for energy applications, CO_2 abatement materials and green corrosion inhibitors.

Recent Publications

1. Winkler D A (2017) Predicting the performance of organic corrosion inhibitors. *Metals*; 7(12): 533.
2. Winkler D A (2017) Biomimetic molecular design tools that learn, evolve and adapt. *Beilstein Journal of Organic Chemistry;* 13: 1288-1302.

Biography

David A Winkler has obtained his degrees in Chemistry, Physics and Chemical Engineering and a PhD from Monash University. He was a Senior Scientist at CSIRO for 30 years then moved to academia. He is interested in translational research aimed at understanding interactions between molecules, materials and biology. He is a Fellow and past Board Chair of the Royal Australian Chemical Institute, a Fellow of the Asian Federation of Medicinal Chemistry; past President of the AFMC and current President of the Federation of Asian Chemical Societies. He is a recent Recipient of the RACI's Adrien Albert award, the American Chemical Society's Herman Skolnik award and the CSIRO Medal in Business Excellence. He has published almost 300 journal articles and book chapters and is an Inventor on 25 patents.

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