(AI) and machine learning (ML) for materials discovery while speeding up the process beyond conventional trial-and-error techniques.

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Abstract:

Climate change challenges & the pressure on the earth crust minerals resources require the discovery of novel & frontier-type compounds. These latter should exhibit diverse multi-functionalities conjugated to a minimum of energy consumption, both during their conception & usage.

Because the number of compounds that can be created from the elements in Mendeleev's periodic table is practically endless and not restricted by the 63 elements initially classified, it is impossible to provide an exact number. A single element, such as carbon, can be used to construct molecules of varied lengths, while other elements can be combined in almost infinite ways to generate distinct substances. Elements can also form numerous compounds.

By employing algorithms to evaluate enormous datasets, spot trends, and forecast novel material properties, artificial intelligence (AI) and machine learning (ML) are revolutionising materials discovery and speeding up the process beyond conventional trial-and-error techniques. These technologies speed up the process of finding new materials for a variety of uses by enabling high-throughput screening of possible materials, computational design of materials with specific features, and autonomous experimentation.

Using High Performance Computational Capabilities (HPCC), this contribution reports on a set of examples related the Energy-Water-Health-Food security nexus in line with the U.N. SDGs landscape. This includes (i) the conversion of CO2 to multi-functional nano-scaled carbonates [1] ,(ii) new generation of nanofluid coolants for heat management [2-3], (iii) Smart nanocoatings for green air conditioning [4], and (iv)bio-inspired nanomaterials for water decontamination [5].

[1]." Room temperature bio-engineered multifunctional carbonates for CO2 sequestration and valorization", M. Maaza et al,
https://www.nature.com/articles/s41598-023-42905-5

[2]."Remarkable thermal conductivity enhancement in Ag—decorated graphene nanocomposites based nanofluid by laser liquid solid interaction in ethylene glycol"
https://www.nature.com/articles/s41598-020-67418-3

[3]. "A novel approach for engineering efficient nanofluids by radiolysis"
https://www.nature.com/articles/s41598-022-14540-z

[4]. "Towards Room Temperature Thermochromic Coatings with controllable NIR-IR modulation for solar heat management & smart windows applications" , M. Maaza et al,
https://www.nature.com/articles/s41598-024-52021-7 ,