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Computational modelling as a value-add in materials design and discovery

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Computer modelling has been identified as a key area of growth worldwide and is increasingly becoming a driving force in the discovery and design of novel materials. Currently, computer simulation methods are influencing all areas of study, with a great impact in condensed matter physics, materials science, chemistry and engineering. With the advancement of computing powers, complex materials and their properties are increasing investigated. Methods at different spatiotemporal scales such as density functional theory, molecular dynamics, energy minimization, many-body perturbation theory, phase field and quantum Monte Carlo to continuum macroscopic approaches are employed to simulate materials for various applications. The search to improve andoptimize properties and structural characterization of materials is a subject of intense scrutiny. However, this has proved challenging because of the complex and preparation-dependent microstructure of many materials. Over the last few years, materials science research have been steadily moving from technique development and determination of fundamental properties towards new materials discovery and design guided by computation, machine learning and data mining, also by a closely tied combination of computational predictions and experimental validation. Thus, thedesign of materials by computation is expected to lead to the discovery of new material and rapid evolution of new materials into products. This talk will broadly highlight recent advances in materials design and discovery, including the application of machine learning techniques in materials science.

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Primary author: Dr MAPHANGA, Rapela (CSIR)

Presenter: Dr MAPHANGA, Rapela (CSIR)

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