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NITheCS Colloquium
Monday, 4 October 2021, 16h00 – 17h00

Prof Regina Maphanga | CSIR

"From density functional theory to machine learning"

ABSTRACT

The discovery of novel materials with high and unprecedented functions is central to technological developments and ultimately human well-being. Computer modelling has increasingly become 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 physics, materials science, chemistry, biology and engineering. With the advancement of computing powers, complex materials and their properties are increasingly investigated. Methods at different spatio-temporal scales spanning from quantum to continuum macroscopic approaches are employed to simulate materials for various applications. Over the past two decades, computational activities in materials science have moved from method development and purely computational studies towards the discovery and design of novel materials guided by modelling results, data mining and machine learning together with a closer collaboration between predictions and experimental validation. This talk will demonstrate how machine learning can be combined with machine learning algorithms to design and predict materials properties.

BIOGRAPHY

Regina Maphanga is a Principal Researcher and Research Group Leader at the Council for Scientific and Industrial Research - Next Generation Enterprises and Institutions Cluster. She is also appointed as NITheCS Associate. Her background is in Physics, specializing in computational modelling of materials.

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