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# Computational modelling and capabilities in metal and alloys

*Monday, 3 December 2018 13:50 (20 minutes)*

The research is based on the development and design of metal alloys with special applications in various industries, from automotive and medical to aeronautical. These alloys have unique properties and behaviour under pressure and temperature conditions. Focus will be on the precious metal, iron-aluminium, titanium and titanium-based systems for shape memory alloys, as well as zirconium-niobium systems. A density functional theory based semi-empirical approach is employed to explore material properties at zero temperature; while molecular dynamics techniques are also carried out to predict the stability, strength, behaviour and the extent of transformation temperature. The overview on computational codes and usage of HPC will be discussed. Furthermore, the advances on machine learning approaches towards titanium cluster development and growth will also be indicated.

## Presenter Biography

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