

# **DFT studies of Iron at extreme temperature and pressure conditions, metal oxides and dopant-induced magnetization in a two-dimensional material**

*Wednesday, 6 December 2023 15:50 (20 minutes)*

We present an overview of some of our recent DFT studies of bulk solid-state systems, of Iron, metal-oxide and alloys, as well as two-dimensional silicene. In particular, we show the applications of x-ray absorption near-edge spectroscopy (XANES) to elucidate the physical and chemical properties of these materials. We show the possibility to induce novel-magnetic properties in silicene through small transition-metal vanadium cluster inclusion. Furthermore, we describe albeit briefly, our recent collaborative work on rare-earth oxides nanostructures. Finally, the central role of high-performance Linux clusters at the CHPC (South Africa) in our computational studies and in facilitating research collaborations within Africa and beyond is discussed.

## **Student or Postdoc?**

No. Not a student nor Postdoc.

**Primary author:** Dr RAJI, Abdulrafiu Tunde (University of South Africa (UNISA))

**Presenter:** Dr RAJI, Abdulrafiu Tunde (University of South Africa (UNISA))

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