

Speaker: [Professor Sébastien Lebègue](#)
Research Professor
National Center for Scientific Research (CNRS)
Nancy, France

Date: Wednesday 4 December 2019

Time: 2.00 pm

Venue: N34 0.04 (Nathan Campus)

Title: **Some recent advances in nanosciences seen through ab initio calculations**

Abstract:

In the field of nanosciences, research on materials has made spectacular progress over the last twenty years. In this talk, I will present, through some examples from recent works, how ab initio calculations can provide a better understanding of the physical and chemical properties of different compounds. In particular, I will discuss the physics of two-dimensional materials, surface physics, and zeolite-type molecular sieves. Finally, some current limits as well as future challenges for ab initio calculations will be described briefly. This talk is for a broad audience including experimentalists.

Short Biography:

After completing a PhD (2000-2003) at the IPCMS-Strasbourg on the development of the GW approximation under the supervision of M. Alouani and a postdoc (2003-2005) in the group of O. Eriksson (Uppsala, Sweden), Sébastien Lebègue obtained a CNRS "Research Fellow" position in Nancy (France) in 2005 and was promoted to Research Professor in 2017. Sébastien Lebègue has published 150 papers in peer-reviewed journals corresponding to approximately 7500 citations, and has a h-index of 36 (source: Google scholar). Sébastien Lebègue is developing and using ab initio methods to understand the electronic structure of solid state compounds, like layered compounds, 2D materials, and surfaces. In particular, Sébastien Lebègue has developed an expertise in methods going beyond standard density functional theory concerning van der Waals forces (semi-empirical corrections to DFT, random phase approximation), excited states properties (GW method, Hubbard-I, Bethe-Salpeter equation) which are often needed to describe in a realistic way the systems of interest.

For enquiries, please contact Dr Tim Gould: t.gould@griffith.edu.au

ALL WELCOME