**Ab initio theory of solid state defect qubits**

Abstract:

Solid-state defects acting as single photon sources and quantum bits are leading contenders in quantum technologies.

Despite great efforts, not all the properties and behaviours of the presently known solid-state defect quantum bits are understood. Furthermore, various quantum technologies require novel solutions, thus new solid-state defect quantum bits should be explored to this end. These issues call to develop ab initio methods which accurately yield the key parameters of solid-state defect quantum bits and vastly accelerate the identification of novel ones for a target quantum technology application.

In this talk, a brief overview about the most recent methods will be shown with emphasizing the complex interplay of electron-phonon coupling in the fine electronic structure of the defects.

The most recent findings on defect qubits and qubit candidates in silicon and other materials will be also presented.