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In search of novel energy materials

The wide spread use of fossil fuels is complicit in the rapid climate change we have witnessed during the past few years. All possible resources to reduce the use of fossil fuels must be explored. At the centre of research in alternative energy technologies is the search for novel materials that can improve the efficiency of solar energy harvesting in solar cells, catalyse hydrogen production and convert waste heat into electricity. Accurate numerical simulations of the properties of compounds is a potential first step in this process. With access to constantly improving computational resources this simulation plays an essential role finding potential compounds. In this talk I'll give an overview of an ab initio numerical simulation approach that enables us to establish whether a compounds is stable, what its physical properties are and its potential as an energy harvester.

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