Development of an automated workflow for well converged DFT calculations for using SIESTA and the AIIDA infrastructure satisfying FAIR data principles

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In the realm of materials science, the advent of advanced computational resources has set the stage for two pivotal ambitions: unravelling the intricate properties of materials and pioneering the discovery of novel ones [1]. Among the myriad of materials, 2D materials stand at the forefront, captivating interest for their versatile applications. This fascination has culminated in the creation of comprehensive databases, cataloguing their properties as predicted by Density Functional Theory (DFT) [2]. These databases are the product of sophisticated high-throughput frameworks designed to streamline and automate computational processes. However, the quest for precision necessitates meticulous attention to ensure that the computational results are not just extensive but also converged and reliable. Despite the progress, there remains ample scope for refining existing data and unveiling new properties yet to be discovered. One of the challenges in high-throughput computational science is adhering to the FAIR principles — ensuring that data are Findable, Accessible, Interoperable, and Reusable [3]. These principles are fundamental in fostering an environment of transparency and reproducibility in scientific research. Moreover, such databases could serve to identify patterns in materials features which could be of great use for material engineering. In particular, we developed an automated workflow utilizing AIIDA [4], DFT simulations package SIESTA [5] and TB2J for exchange constant calculations [6] to compute bandgap, band structure plots, and exchange constant [6]. These calculations will enable us the possibility to compute the Curie temperature of 2D magnetic materials through Monte Carlo methods. We expect this work will serve to identify the critical features required to further increase the Curie temperature of 2D magnets thus opening a new gate for low-power low-dimensional magnetic memories.

References

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