ID de Contribution: **33** Type: **Non spécifié**

A Database of Spin Splittings in 2D Materials

mardi 13 septembre 2022 14:30 (20 minutes)

Abstract

The development of spintronic devices demands the existence of materials with some kind of spin splitting (SS). With de the advance in the development of 2D materials in the last two decades, this family of compounds brought great opportunities for applications in spintronic devices. Finding the best materials for this assignment, however, is a challenging task. To advance the understanding of this subject, we build a database of ab initio calculated SS in 2D materials. More than that, we propose a workflow for materials design integrating an inverse design approach and a Bayesian inference optimization. We use the prediction of SS prototypes for spintronic applications as an illustrative example of the proposed workflow. The prediction process starts with the establishment of the design principles (the physical mechanism behind the target properties), that are used as filters for materials screening, followed by density functional theory (DFT) calculations. Applying this process to the C2DB database, we identify and classify 358 2D materials according to SS type at the valence and/or conduction bands. The SS type can be either Rashba, Dresselhaus, Zeeman, or high order. The Bayesian optimization captures trends that are used for the rationalized design of 2D materials with the ideal conditions of band gap and SS for potential spintronics applications. Our workflow can be applied to any other material properties. In this talk, we will explain the construction process for the database and illustrate how it can be used for further studies.

References

[1] Nascimento, G.M., Ogoshi, E., Fazzio, A., Acosta, C. M., and Dalpian, G. M.. High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds. Scientific Data 9, 195 (2022).

Orateur: Prof. M. DALPIAN, Gustavo (Center for Natural and Human Sciences - Federal University of ABC)

Classification de Session: Plenary