**Elevating Material Simulations with Open Source – From Consumer to Contributor**

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Computational Material Science is a well established field in South Africa. A great many presentations during the annual conference of the South African Institute of Physics are dedicated to materials simulations with Density Functional Theory. There are however few contributions which go beyond the application of existing codes and algorithms.
This can be attributed in part to the perceived high obstacles from closed source programmes and programmes which are badly documented and difficult to understand. In this contribution I would like to introduce the open source DFT code GPAW, which is written largely in Python. It is not only comparable in features to expensive closed source software like VASP, it also has some unique features. More importantly for this contribution, GPAW is very easy to read and modify.
I will showcase this using the electron-phonon coupling and Raman spectroscopy codes I contributed to the GPAW package, which is documented in our lasted review paper "GPAW: An open Python package for electronic structure calculations" published in The Journal of Chemical Physics ( https://pubs.aip.org/aip/jcp/article/160/9/092503/3269902 ) and has been used to predict the Raman spectrum if a large number of 2D materials.
It is my hope to motivate more South African researchers to participate in software development to raise our global profile and give back to the community.

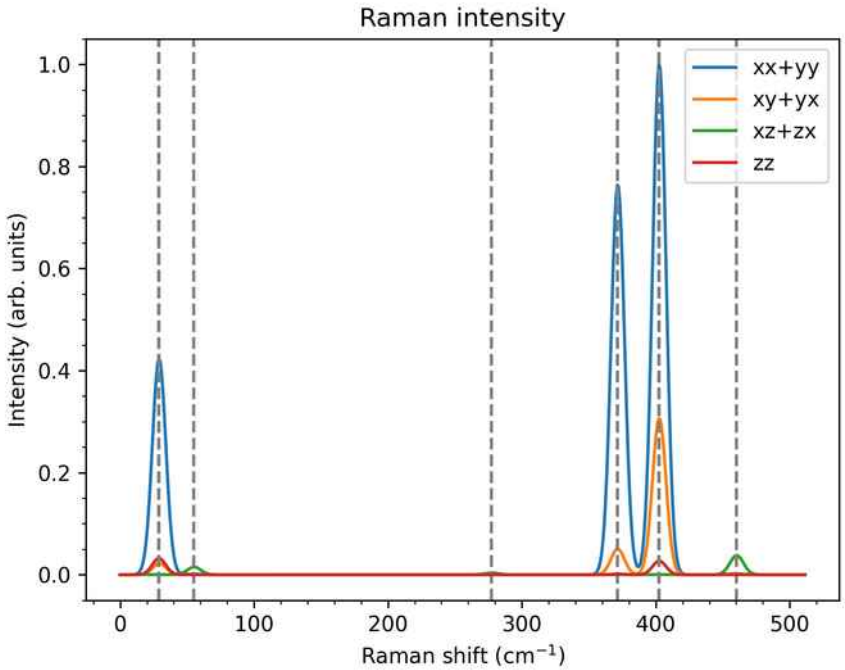


*Figure 1: MoS2 Raman spectrum as calculated with GPAW.*