Contribution ID: **77** Type: **Poster**

【194】High-throughput GW Calculations

Tuesday, 31 August 2021 19:23 (1 minute)

The goal of our work is generating an automated workflow for calculating quasi-particle band gaps within the so-called GW method. The resulting protocol is applied to a large materials dataset of about 100 materials, from binary to quaternary compounds. Conventional approaches of performing these calculations require significant amounts of computational resources and user interaction, inhibiting efficient investigation of large datasets or high-throughput procedures. To avoid this, we employ a basis set extrapolation method for correcting errors arising due to finite energy cut-offs and show that it is possible to design practical workflows, which can be implemented in existing workflow managers easily and produce high-accuracy data while requiring minimal user interaction.

Primary authors: Prof. FRANCHINI, Cesare (University of Vienna); ELLINGER, Florian (University of Vienna)

Presenter: ELLINGER, Florian (University of Vienna)

Session Classification: Poster Session

Track Classification: Condensed Matter Physics (KOND)