

Automated program for *ab initio* calculations

Ab initio calculations based on the density functional theory (DFT) become a vital tool in materials science for understanding and predicting material properties. However, it requires in-depth knowledge on underlying theories and enough experience to produce reliable data. Recently, several automation utilities have been developed to accelerate data production but they still assume that users are familiar with technical details. Here, we introduce a full-fledged automation code running a DFT program. The package requires only structure information from the user and provides a highly accurate band structure, band gap, effective mass, density of states and dielectric constant for the given structure. As a result, anyone can run DFT program without any background knowledge using the package.

