effmass: An effective mass package

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Summary

Many semiconductor properties depend on the response of electrons to an external pertubation. This perturbation could take the form of an electric field, change in temperature or an applied lattice stress. In a crystal, this response depends on the interaction of the electrons with a periodic potential. The effective mass approximation assumes that the response of an electron in a periodic potential is equivalent to that of a free electron with a renormalised mass (called the "effective mass"). This makes the effective mass a critical parameter in models for the optical and transport properties of a semiconductor.

The effective mass has a number of definitions, depending on the perturbation under consideration. The conventional definition of effective mass is inversely proportional to the second derivative of electron energy with respect to electron momentum (N. W. Ashcroft 1976, 227). This allows the effective mass to be easily calculated from *ab-initio* band structures, and there are existing codes which have implemented this (A. Fornari 2012 ; B. Morgan 2018).

We must approximate the band structure with a parabola for the previous definition to be valid (V. Ariel 2012). However, this approximation breaks down when there is a high concentration of electrons in the material - when, for example, the material is doped or excited under a laser. Instead, we can then approximate the band structure with the Kane quasi-linear dispersion (E. O. Kane 1957), and the definition of effective mass is adapted accordingly.

`effmass` (L. D. Whalley 2018) is a Python 3 package for calculating various definitions of effective mass from the electronic bandstructure of a semiconducting material. It contains a core class that calculates the effective mass and other associated properties of selected band structure segments. `effmass` also contains functions for locating band structure extrema, calculating the Kane quasi-linear dispersion parameters and plotting approximations to the true dispersion. Parsing of electronic structure data is faciliated by the `vasppy` (B. Morgan 2018) package.

Acknowledgements

References

A. Fornari, C. Sutton. 2012. "Effective Mass Calculator." GitHub. https://github.com/afonari/emc.

B. Morgan. 2018. "vasppy: A Python suite for manipulating VASP input and output." Zenodo. https://doi.org/10.5281/zenodo.1263753.

E. O. Kane. 1957. "Band Structure of Indium Antimonide." *Journal of Physics and Chemistry of Solids* 1 (4): 249–61. https://doi.org/10.1016/0022-3697(57)90013-6.

L. D. Whalley. 2018. "effmass: An effective mass calculator." Zenodo. http://dx.doi.org/10.5281/zenodo.1285137.

N. W. Ashcroft, N. D. Mermin. 1976. *Solid State Physics*. Saunders College.

V. Ariel, A. Natan. 2012. "Effective mass and the Energy-Mass relationship." arXiv. https://arxiv.org/abs/1205.3995.