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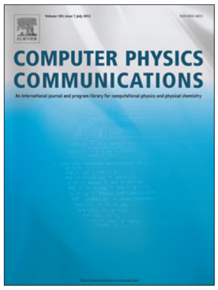

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Kubo-Greenwood Electrical Conductivity Formulation and Implementation for Projector Augmented Wave Datasets

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Abstract

As the foundation for a new computational implementation, we survey the calculation of the complex electrical conductivity tensor based on the Kubo-Greenwood (KG) formalism (J. Phys. Soc. Jpn. **12**, 570 (1957); Proc. Phys. Soc. **71**, 585 (1958)), with emphasis on derivations and technical aspects pertinent to use of projector augmented wave datasets with plane wave basis sets (Phys. Rev. B **50**, 17953 (1994)). New analytical results and a full implementation of the KG approach in an open-source Fortran 90 post-processing code for use with Quantum Espresso (J. Phys. Cond. Matt. **21**, 395502 (2009)) are presented. Named KGEC ([K]ubo [G]reenwood [E]lectronic [C]onductivity), the code calculates the full complex conductivity tensor (not just the average trace). It supports use of either the original KG formula or the popular one approximated in terms of a Dirac delta function. It provides both Gaussian and Lorentzian representations of the Dirac delta function (though the Lorentzian is preferable on basic grounds). KGEC provides decomposition of the conductivity into intra- and inter-band contributions as well as degenerate state contributions. It calculates the dc conductivity tensor directly. It is MPI parallelized over k-points, bands, and plane waves, with an option to recover the plane wave processes for their use in band parallelization as well. It is designed to provide rapid convergence with respect to **k**-point density. Examples of its use are given.

Keywords: Electron transport, Kubo-Greenwood, electrical conductivity, Kohn-Sham density functional theory, plane wave, projector augmented wave

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