

Abstract Submitted
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**Kubo-Greenwood Electric Conductivity Tensor:
Essentials and Open-source Implementation¹** LAZARO CALDERIN,
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of Florida — We survey the essentials for calculation of the complex electric con-
ductivity tensor based on the Kubo-Greenwood (KG) formalism, then discuss our
new implementation of a KG post-processing tool for Quantum Espresso. The mo-
tivating physical problem is computational characterization of warm dense matter.
Solutions to both formal and technical problems implicit in the use of Projector
Augmented Wave datasets and a plane wave basis will be discussed, especially in
the context of simulations of materials in extreme conditions. A full implementation
in an open-source Fortran 90 code and illustrative results from it will be presented.

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