

Abstract Submitted
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***Ab initio* Optical Absorption by A Simple and Efficient Method:
Single Excitation Configuration Interaction After Downfolding** KAZUMA
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Dept. of Physics, University of Tokyo — We present a simple and efficient *ab initio*
method for calculating electronic excited states and optical absorption spectra of
solids. The method is based on a single-excitation configuration-interaction calcu-
lation after downfolding to model Hamiltonians represented by maximally-localized
Wannier functions. Single-excitation configurations are crucially important in eval-
uating a linear absorption, because they can describe a so-called excitonic effect;
interactions in electron-hole pairs generated by excitations. A test was performed
for a semiconductor GaAs, and detailed analyses for the resulting spectra and single-
excitation many-body wavefunctions are presented. This work is supported by a
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