Abstract Submitted
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GW-based *ab initio* downfolding aiming at strongly correlated electron system[1] KAZUMA NAKAMURA, Dept. of Applied Physics, Univ. Tokyo, TAICHI KOSUGI, Dept. of Physics, Univ. Tokyo, YOSHIHIDE YOSHIMOTO, ISSP, Univ. Tokyo, RYOTARO ARITA, RIKEN, MASATOSHI IMADA, Dept. of Applied Physics and JST-CREST, Univ. Tokyo — Aiming at *ab initio* description of real complex systems under effects of strong electron correlations, we develop a GW-based downfolding scheme formulated in the plane-wave basis set. Our method is successfully applied to organic conductors, the family of (BEDT-TTF)$_2$X. At the heart of our downfolding scheme lies utilizing the energy hierarchy of the system [1]: The low-energy hierarchy near the Fermi level ($\varepsilon_f \pm 2 \sim 3$ eV) determines physics while is affected by the remaining high-energy part of hierarchy. We renormalize the high-energy part into low energy, based on the GW scheme. The renormalization generates a low-energy model characterized by renormalized transfers and effective screened Coulomb/exchange interactions, having frequency dependence arising from retarded screening by eliminated high-energy electrons. Thus, the low-energy frequency-dependent effective model is mapped out from the whole high- plus low-energy system in an *ab initio* procedure. [1] F. Aryasetiawan *et al.*, Phys. Rev. B **70**, 19514 (2004); I. V. Solovyev and M. Imada, *ibid.* **71**, 045103 (2005).

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