Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

New method for calculating the optical absorption spectrum for solids using the transcorrelated method MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo, ISSP, The University of Tokyo — *Ab initio* calculation of an accurate optical absorption spectrum for solids is a challenging problem, and various methods are proposed for this purpose, such as TDDFT using new functionals and GW+BSE. In this study, we propose a new method for calculating the optical spectra, using the transcorrelated (TC) method[1-6], which is one of the promising wave-function theories. In the TC method, the total wave function is approximated as the Jastrow-Slater-type wave function, and the many-body Hamiltonian is similarity-transformed by the Jastrow factor. Then we solve an SCF equation and optimize one-body orbitals in the Slater determinant with a relatively low computational cost.[6] For excited-state calculations, we use configuration interaction singles (CIS) for the TC method, and will present an optical absorption spectrum of LiF calculated with this method. [1] S. F. Boys and N. C. Handy, Proc. R. Soc. London Ser. A 309, 209 (1969). [2] S. Ten-no, Chem. Phys. Lett. 330, 169 (2000). [3] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. 119, 10015 (2003). [4] R. Sakuma and S. Tsuneyuki, J. Phys. Soc. Jpn. 75, 103705 (2006). [5] H. Luo, J. Chem. Phys. 133, 154109 (2010). [6] M. Ochi, K. Sodeyama, R. Sakuma, and S. Tsuneyuki, J. Chem. Phys. 136, 094108 (2012).

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Date submitted: 09 Nov 2012 Electronic form version 1.4