

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Ground state properties of simple solids from GW calculations.

ANDREY KUTEPOV, SERGEY SAVRASOV, Department of Physics, University of California, Davis, California 95616, USA — A novel self-consistent implementation of Hedin's GW perturbation theory is presented. This finite-temperature implementation uses Hartree-Fock wave functions to represent Green's function. Hartree-Fock equations are solved with full potential linear augmented plane wave (FLAPW) method at each iteration of a self-consistent cycle. With our approach we are able to calculate total energy and the ground state properties. As an example, the ground state properties of Na, Al, Si, and GaAs obtained with our new code are presented.

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Date submitted: 19 Nov 2008

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