Local self-energy approach for electronic structure calculations
NIKOLAY ZEIN, SERGUEI SAVRASOV, New Jersey Institute of Technology,
GABRIEL KOTLIAR, Rutgers University — We implement method for electronic
structure calculations which utilizes GW approximation combined with dynamical
mean field theory (DMFT). To study the locality of electronic self-energy operator
we compared all the relevant quantities as obtained in both R and k spaces. Con-
vergence of the exchange diagram as well of the correlational part for the self-energy
within GW and its first vertex correction are checked as functions of cutoff radius
in the real space. Our approach permits calculations beyond GW in a controllable
manner. Full self-consistency with respect to Green functions is implemented which
erases information on the starting point given either by LDA or Hartree-Fock ap-
proximations. Results obtained for a number of covalent and ionic semiconductors
will be discussed and compared with various existing calculations and experiments.
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