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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. Convergence 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 approximations. Results obtained for a number of covalent and ionic semiconductors will be discussed and compared with various existing calculations and experiments. Work supported by NSF, DOE and CMSN.

Nikolay Zein
New Jersey Institute of Technology

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