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Quasiparticle self-consistent GW method applied to f systems MARK VAN SCHILFGAARDE, ATHANASIOS CHANTIS, TAKAO KOTANI, Arizona State University, ANDRE PETUKHOV, South Dakota Tech — We have applied the recently-developed quasi-particle self-consistent GW method (QPscGW) to several f systems, Gd, GdN, GdAs, ErAs, and CeO2. The QPscGW is desigened to determine the best independent particle picture; it can cover rather wide-range of materials, semiconductor to transion metal oxides with acceptable accuracy [1] [2] without any parameters. We found that QPscGW gives reasonable description of the f level positions and exchange splitting, though it predicts unoccupied f levels a little too high. In addition, the Fermi surface analysis shows that SdH frequencies and carrier concentration are in good agreement with available experimental data. [1] Mark van Schilfgaarde, Takao Kotani, and Sergey V. Faleev, cond-mat/0510408 [2] A. N. Chantis, Mark van Schilfgaarde, Takao Kotani, cond-mat/0508274

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