Quasiparticle self-consistent GW method applied to f systems
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Arizona State University, ANDRE PETUKHOV, South Dakota Tech — We have
applied the recently-developed quasi-particle self-consistent GW method (QPsc\textit{GW})
to several f systems, Gd, GdN, GdAs, ErAs, and CeO2. The QPsc\textit{GW} is designed
to determine the best independent particle picture; it can cover rather wide-range
of materials, semiconductor to transition metal oxides with acceptable accuracy [1]
[2] without any parameters. We found that QPsc\textit{GW} 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.