

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Combined semilocal exchange potential with dynamical mean-field theory** LI HUANG, HAIYAN LU, China Academy of Engineering Physics — The modern semilocal exchange potential is an accurate and efficient approximation to the exact exchange potential of density functional theory. We tried to combine it with the dynamical mean-field theory to derive a new first-principles many-body approach for studying correlated electronic materials. As a paradigm, this approach was employed to investigate the electronic structures and optical properties of strongly correlated ionic insulator YbS. Compared to the regular density functional theory plus dynamical mean-field theory which surprisingly failed to give an insulating solution, the new approach correctly captured all of the important characteristics of YbS. Not only an energy gap between a fully occupied Yb-4*f* state and an unoccupied conduction band, but also an absence of Drude peak in the optical conductivity  $\sigma(\omega)$  were successfully reproduced.

Li Huang  
China Academy of Engineering Physics

Date submitted: 09 Nov 2016

Electronic form version 1.4