



北京理工大学
Beijing Institute of Technology

“21世纪学科前沿”系列学术报告

First-principles approaches to electronic band structure of materials

2017 5 15 15 00

118

is a b a a d
 n b a b n b
 d b a . n b b p
 n b p n o a g g
 n b w -w d g n 1]. Aa b
 b b d a b n s b b g n n
 b th d p a . n b b d a b
 b n w w b a d a n a b
 a d p a b d n -d p p n b
 W p [2] d p a p n a p b a
 p . d b b d b a b a g b a
 b p b b d a b b n n w
 th a ab n d g d d -b
 n . h b w l w p o e b b n
 a d b s -p d a p b b d
 a b n g n a W p n b d
 th w (AV n [2] a p th Bk -
 d p [3] a a k d n p b b d a
 b n n d g a g p b b
 d a b d th .

- [1] Hg, GCh, , 24, 910 (2012).
- [2] Hg, FBa, PRB, , 93, 115203 (2016).
- [3] Hg, JCh, 138, 134115 (2013).