



$$V_c(r, r') = \alpha \sum_i \frac{\psi_i(r) (\mu |r - r'|) \psi_i^*(r)}{|r - r'|}. \quad (2)$$

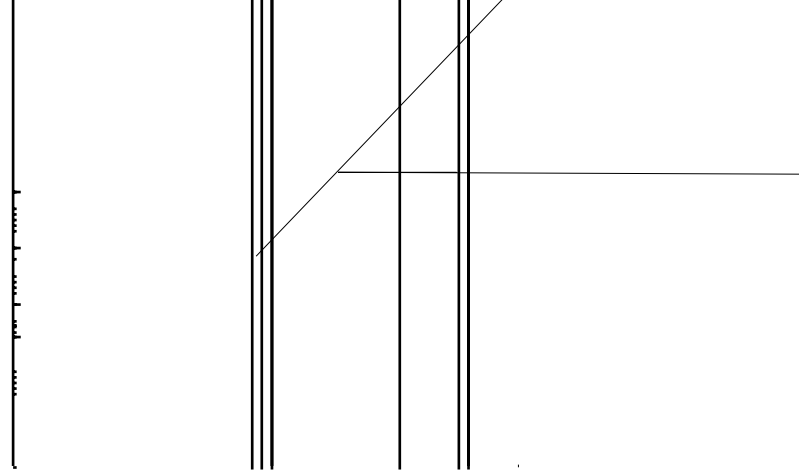
A a  $\mu=0.2$   $\mu=0$   $\mu=0.40$   $\mu=0.25$   $\mu=0.16$   $\mu=0.12$   $\mu=0.21$   $\mu=0.1$   $\mu=0.09$   $\mu=0.22$

T, PBE, S, HF, HSE, PBE, (HSE-25/HSE-40), DFT, HF, HF-DFT, Z O, LDA, LDA-

(2), S, HF, PBE, (HSE-25/HSE-40), DFT, HF, HF-DFT, Z O, LDA, LDA-

Z O, <sup>9,22</sup>

Table 1. Calculated band structures of Ta<sub>2</sub>O<sub>5</sub> using different exchange-correlation functionals (GGA, PBE, HSE-25, and HSE-40) and the experimental data (II).



4( )  $V_Z$   $I$   $X$   $a$   $3R^{32}$   $E$   $LDA+U$   $22$   $O$   $Z$   $F_V$ .  
 4(a) 4( ).

$V^0$   $+0.85$   $V$   $X$   $a$   $+1$   $V$   
 HSE  $La^9$   $a$   $1.0$   $V$   $O$   $a^{16}$   $I$   $4$   $V$   
 Ja  $22$   $T$   $+0.85$   $V$   $10^{19}$   $a$   $700$   $C$   $-$   
 $28$   
 ( )  $T$   $a$   $a$   $(0/++)$   $V_O$   $E_V$   
 $HSE-40$   $a$   $X$   $a$   $a$   $a$   $E_V$   
 $+(2.2$   $2.3)$   $V$   $Ja$   $22$   $I$   $a$   $a$   $a$   
 HSE-25  $a$   $E_V+1.7$   $V$   $GW$   $a$   $a$   $a$   
 HSE-25 (R  $23$ )  $E_V+1.7$   $V$   $1.4$   $V$   
 (GW  $GGA+U$ )  $T$   $a$   $a$   $a$   
 LDA+C  $La^9$   $a$   $a$   $(0/++)$   $a$   $E_V$   
 $+1.3$   $V$ .

**E. Assessment of previous LDA-corrected calculations**

$T$   $a$   $a$   $a$   $-LDA$   $a$   
 $X$   $HSE$   $GW$   $a$   $a$   $a$   
 $LDA-$   $a$   $a$   $a$   
 $(C=C)$   $E$   $a$   $W$   $GGA-C$   
 $Ja$   $Va$   $Wa$   $22$   $a$   $a$   
 $U$   $Z$   $3d$   $a$   
 $U (=6$   $V)$   $E_V$   $0.7$   $V$   $a$   $-$   
 $(CBM)$   $T$   $a$   $a$   $a$   
 $LDA-C$   $a$   $a$   $a$   $a$   $a$   
 $W$   $a$   $a$   $a$   $a$   
 $-LDA$   $a$   $a$   $a$   $a$   
 $( )$   $F_V$   $5$   $a$   $Ta$   $II$   $a$   $X$   $a$   
 $V_O$   $a$   $a$   $LDA-C$   $a$   $T$

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