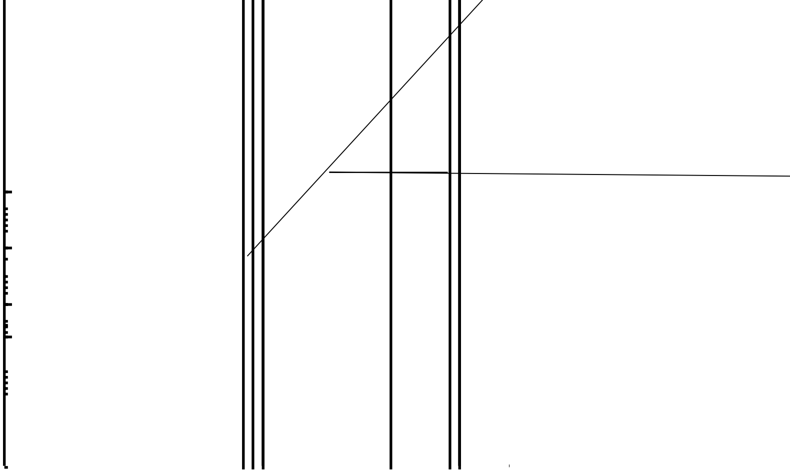
$$V(r,r') = \alpha\sum_{i}\frac{\psi_i(r)\quad(\mu|r\quad r'|)\psi_j^*(r)}{|r\quad r'|}. \qquad (2)$$

A a a a a a μ=0.2 1 a a- a .[15] T PBE a μ=0 E . (2). S a a HF a HSE a a , a α PBE a 0.25, a a a ~0.40 a a Z O.[16] W a (HSE-25/HSE-40) a . F 1 a X a DFT a , a a a HF a $(r\quad r')$. T a a a Z O.[12,16 21] H , a a HF-DFT a HF a (F . 1) a Z O, a a a a a a . T a a a a a a a , a LDA. T a a LDA- Z O,[9,22]

a (X, PBE , HSE-25, a HSE-40) Ta II,
a a GGA ( )



4( ) a a X a a a V_Z . I a . T - a a .[31,32] E LDA+U a .[22] O a , a V_O a a a Z , F . 4(a) 4( ).

E. Assessment of previous LDA-corrected calculations

T a a a -LDA X, HSE, GW a a LDA- , a - . W GGA-C (C=C). E a LDA+U Ja a Va Wa[22] a a , a a U Z 3d a a , a a . La[9] - a a U (=6 V) E_V 0.7 V, a - a a (CBM). T a LDA-C a a . W a a a -LDA a a , : ( ) F . 5 a Ta II a X a V_O a a LDA-C . T

a V^0 +0.85 V X a +1 V HSE a La[9] a a 1.0 V O a.[16] I a 4 V Ja .[22] T +0.85 V a a a a 10^{19} ^{3} a 700 C, - .[28]

( ) T a a (0/++) V_O : HSE-40 a X, a a a E_V +(2.2 2.3) V, Ja .[22] I a , a HSE-25 a E_V+1.7 V, GW a a HSE-25 (R . 23) E_V+1.7 V 1.4 V (GW GGA+U). T a LDA+C La[9] a a (0/++) a E_V +1.3 V.

*J @ . a .a .

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