

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

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, ^{9,22}

Table 1. Calculated band structures of Ta₂O₅ using different exchange-correlation functionals (GGA, PBE, HSE-25, and HSE-40) and the experimental data (II).

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