Specific Features of Electronic Structures and Optical Susceptibilities of Molybdenum Oxide

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Supporting information

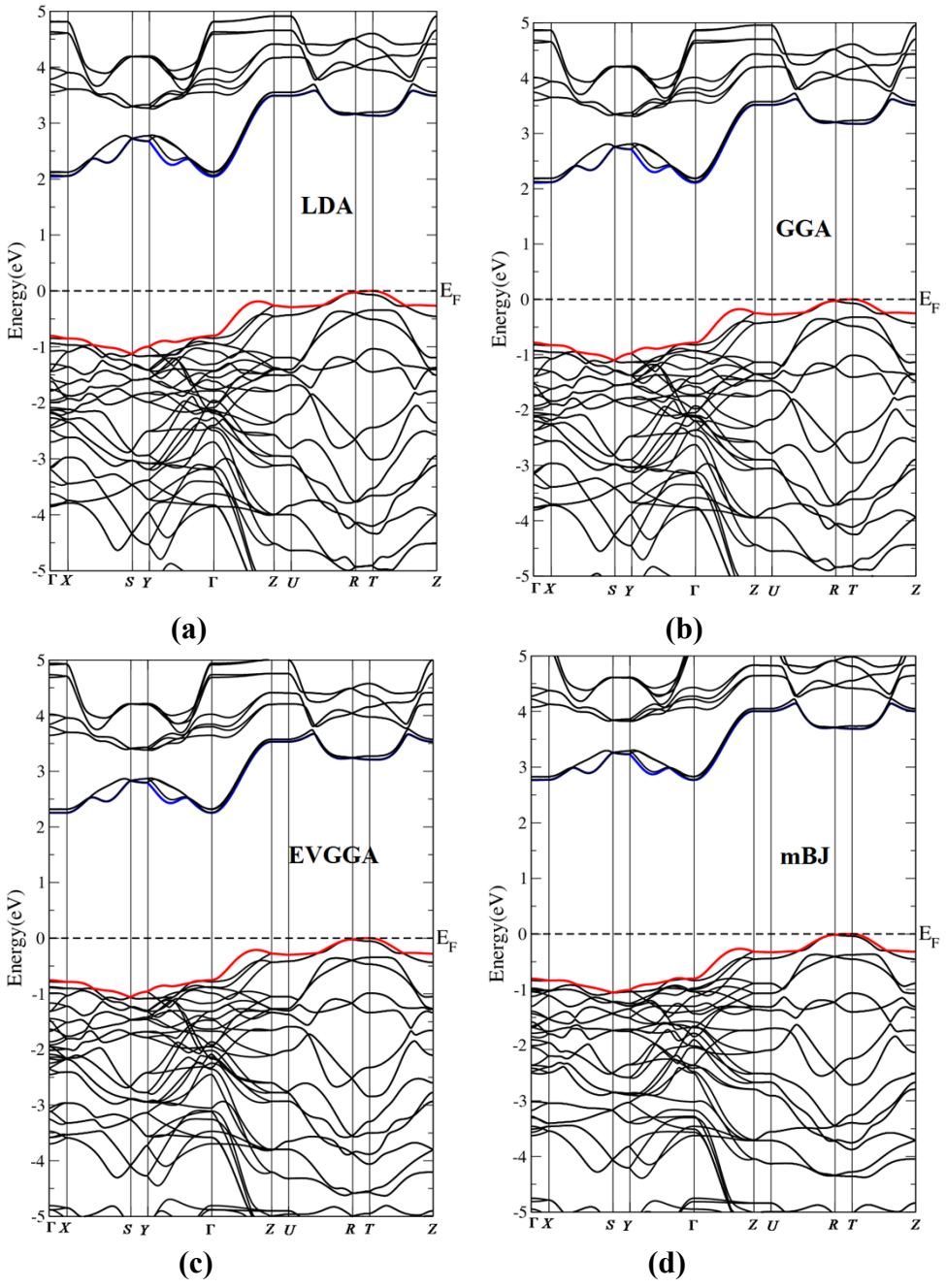

Fig. S1: The calculated electronic band structure of $\alpha - MoO_3$ using; (a) *LDA*; (b) *GGA*; (c) *EVGGA*; (d) *mBJ*.

Table S1: The calculated energy band gaps in comparison with the experimental value.

Eg (eV)				
LDA	**GGA**	**EVGGA**	**mBJ**	**Eg (Exp.)**
2.050*	2.114*	2.257*	2.81*	3.03[a], 3.1[b]

*This work
[a]Ref. 25, [b]Ref. 6

Table S2: The calculated $\varepsilon_1^{xx}(0)$, $\varepsilon_1^{yy}(0)$, $\varepsilon_1^{zz}(0)$ and $\varepsilon_1^{av}(0)$.

	LDA	**GGA**	**EVGGA**	**mBJ**
$\varepsilon_1^{xx}(0)$	5.95	5.85	5.54	4.80
$\varepsilon_1^{yy}(0)$	5.61	5.49	5.24	4.32
$\varepsilon_1^{zz}(0)$	6.30	6.15	5.82	5.03
$\varepsilon_1^{av}(0)$	3.87	3.79	3.6	3.05