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Supporting Information

Phase Polymorphism and Electronic Structures of $TeSe_2$

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Table S1. Calculated structural properties for $M_H \rightarrow H_{\gamma T}$ and $M_H \rightarrow M_{\beta\alpha}$ phase transformations. Lengths are in units of Å.

Phase	$l_{Te\text{-}Te}^1$, $l_{Te\text{-}Te}^2$	$l_{Se\text{-}Se}^1$, $l_{Se\text{-}Se}^2$	$l_{Te\text{-}Se}^1$, $l_{Te\text{-}Se}^2$
M_H	4.17	2.49	2.66
	4.25	3.35	3.32
$H_{\gamma' T}$	4.00	3.54	2.80
	3.86	4.00	2.83
$H_{\gamma T}$	3.99	3.50	2.84
	3.99	3.99	2.84
$M_{\beta\alpha'}$	4.05	2.52	2.70
	4.04	3.35	3.24
$M_{\beta\alpha}$	4.16	2.49	2.66
	4.24	3.35	3.21

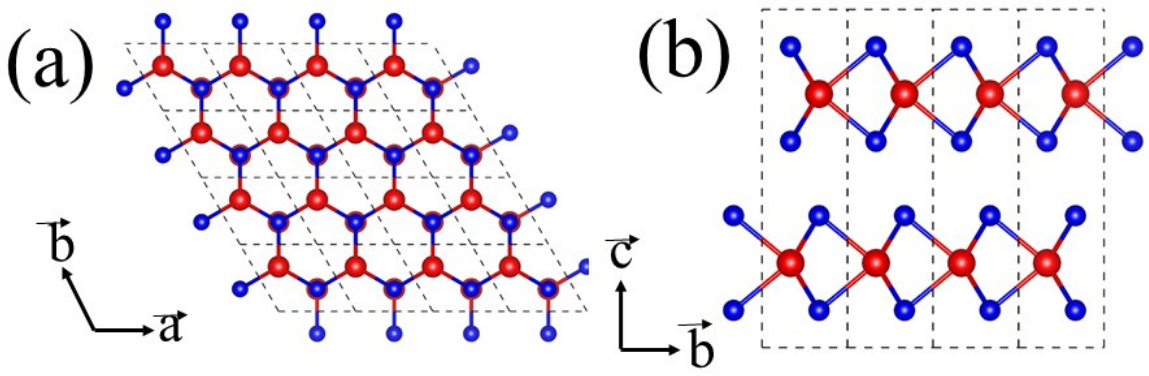


Figure S1. Chemical structure of $TeSe_2$ in the $H_{\varepsilon H}$ phase in (a) top and (b) side views. The red and blue balls represent Te and Se atoms, respectively.

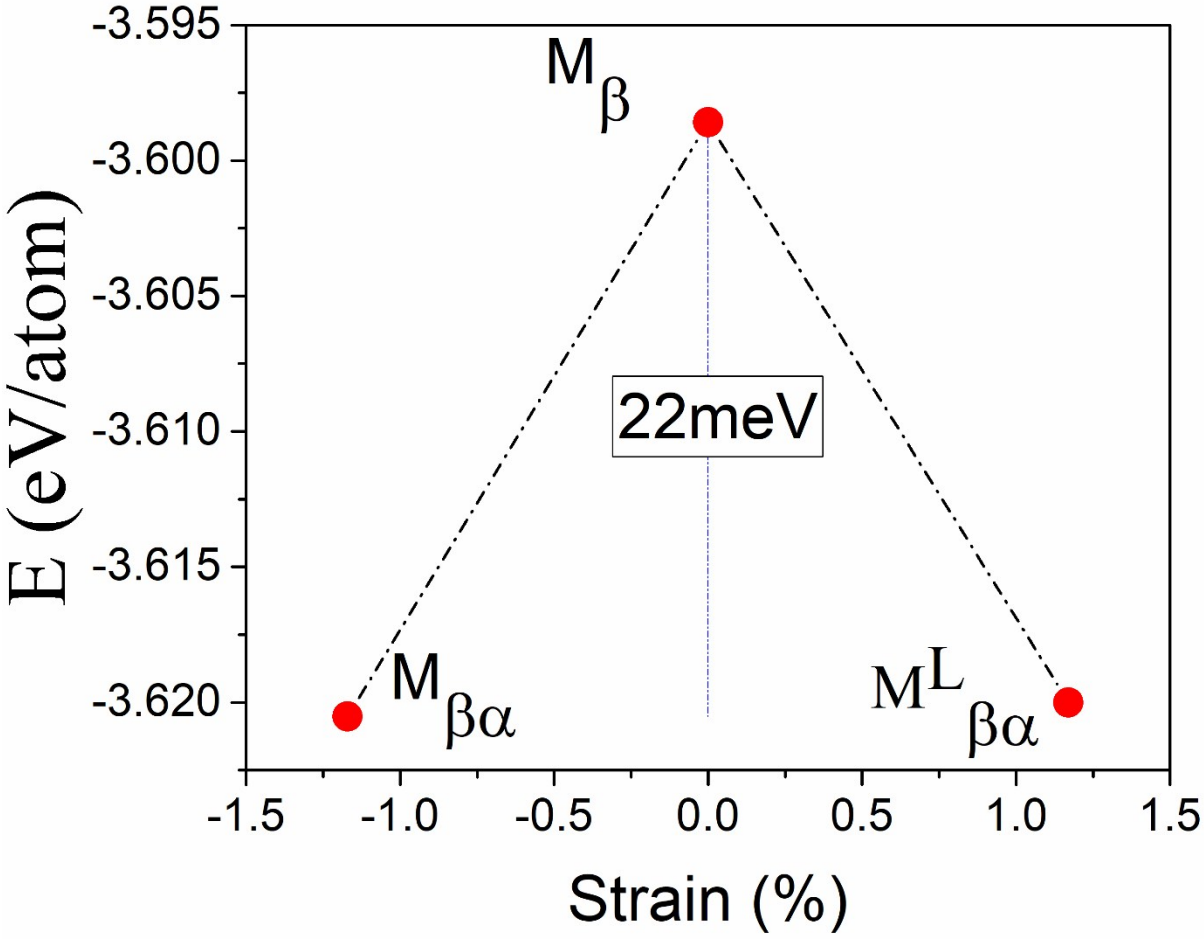


Figure S2. Phase transformations between $M_{\beta\alpha}$ and $M^{L}_{\beta\alpha}$ under shear stress, where $M^{L}_{\beta\alpha}$ is a mirror image of $M_{\beta\alpha}$.

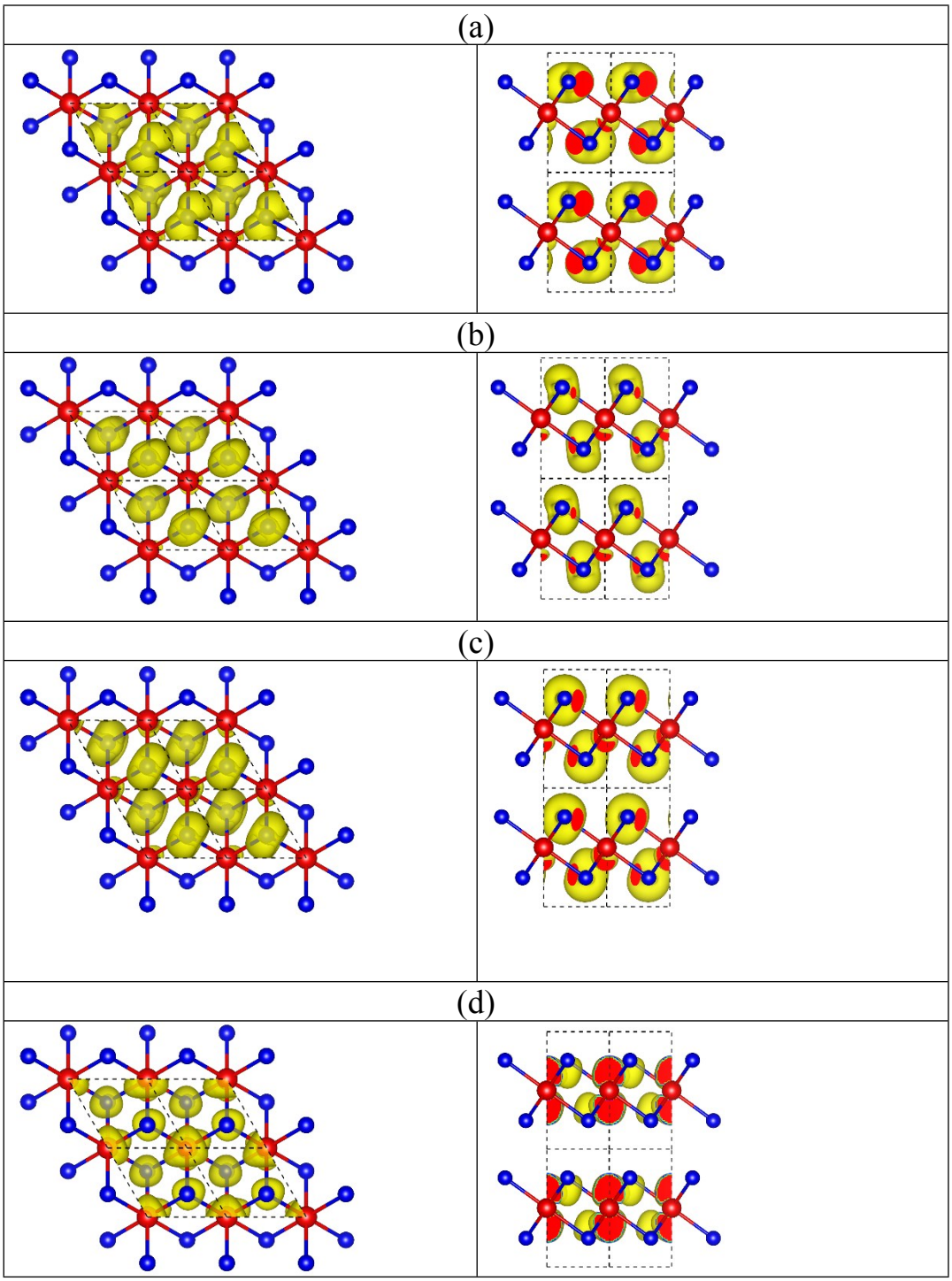
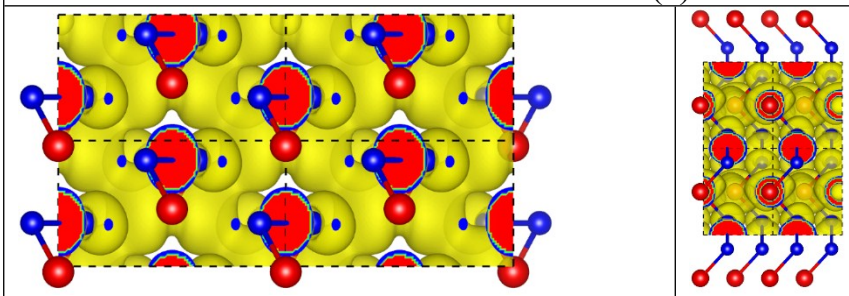
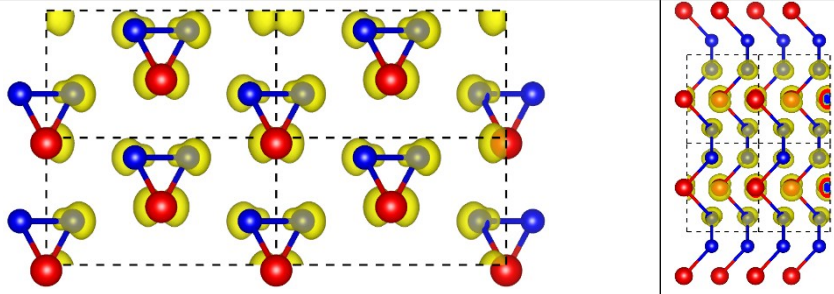


Figure S3. Two different views of the charge density plots of the valence band in the H_{VT} phase at K' (Γ→K) (a), A' (A→L) (b) and A" (A→H) (c) points. Similar plots are also shown for the conduction band at the A point (d). The charge density visualization is shown with isosurface of 0.002 eÅ^{-3}.The red and blue balls represent Te and Se atoms, respectively.

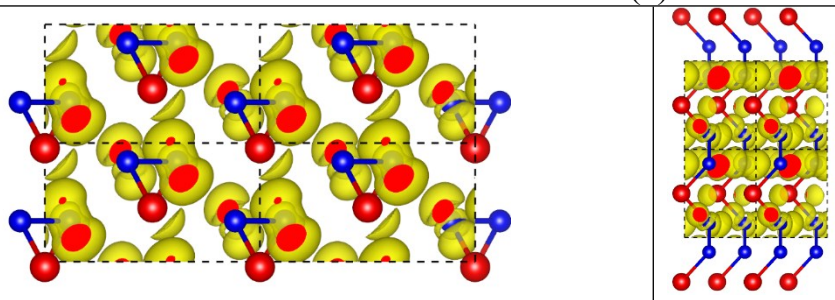
(a)



(b)



(c)



(d)

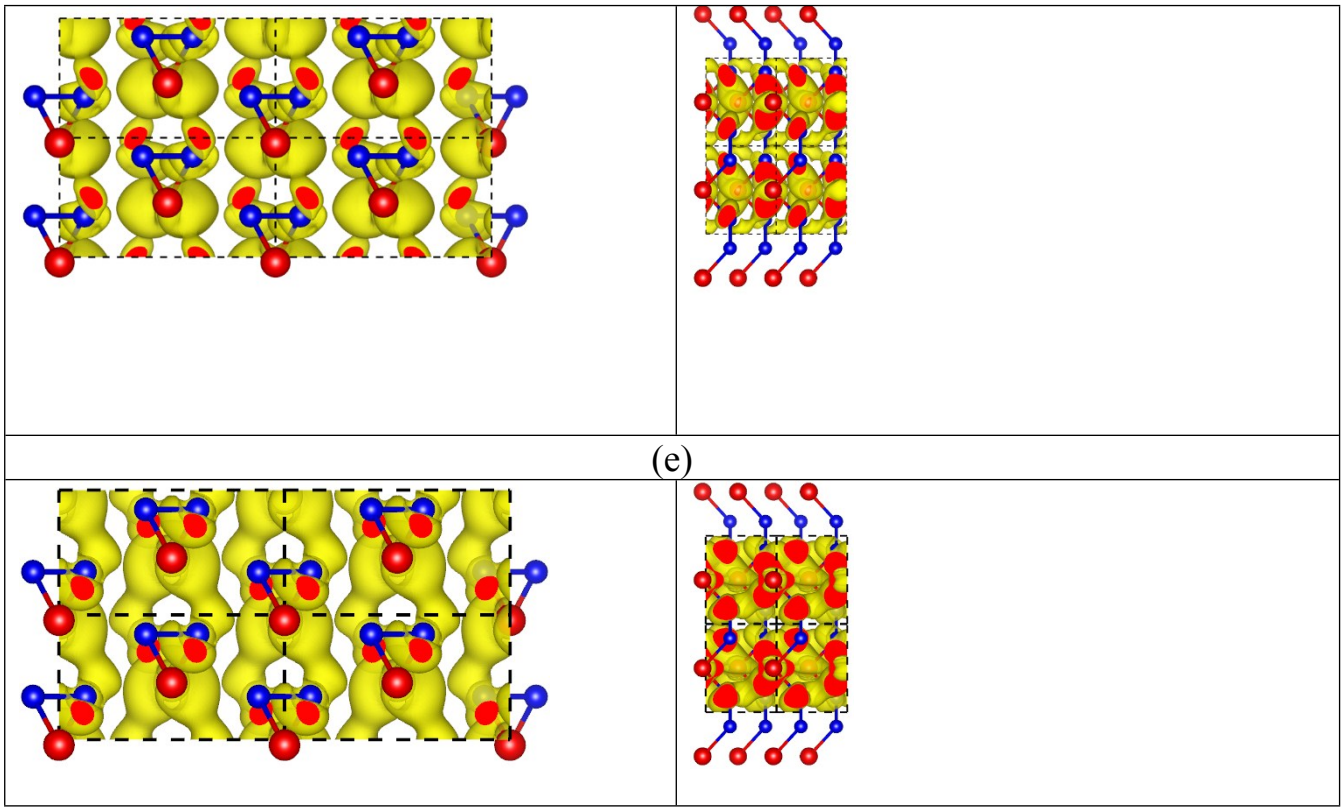


Figure S4. Two different views of the charge density plots of the valence band in M_H phase at Z (a), D' (B→D) (b), and E (c) points. Similar plots are also shown for the conduction band at at Z' (Z→Γ) (d) and D' (B→D) (e) points. The charge density visualization is shown with isosurface of 0.0003 eÅ^{-3}. The red and blue balls represent Te and Se atoms, respectively.

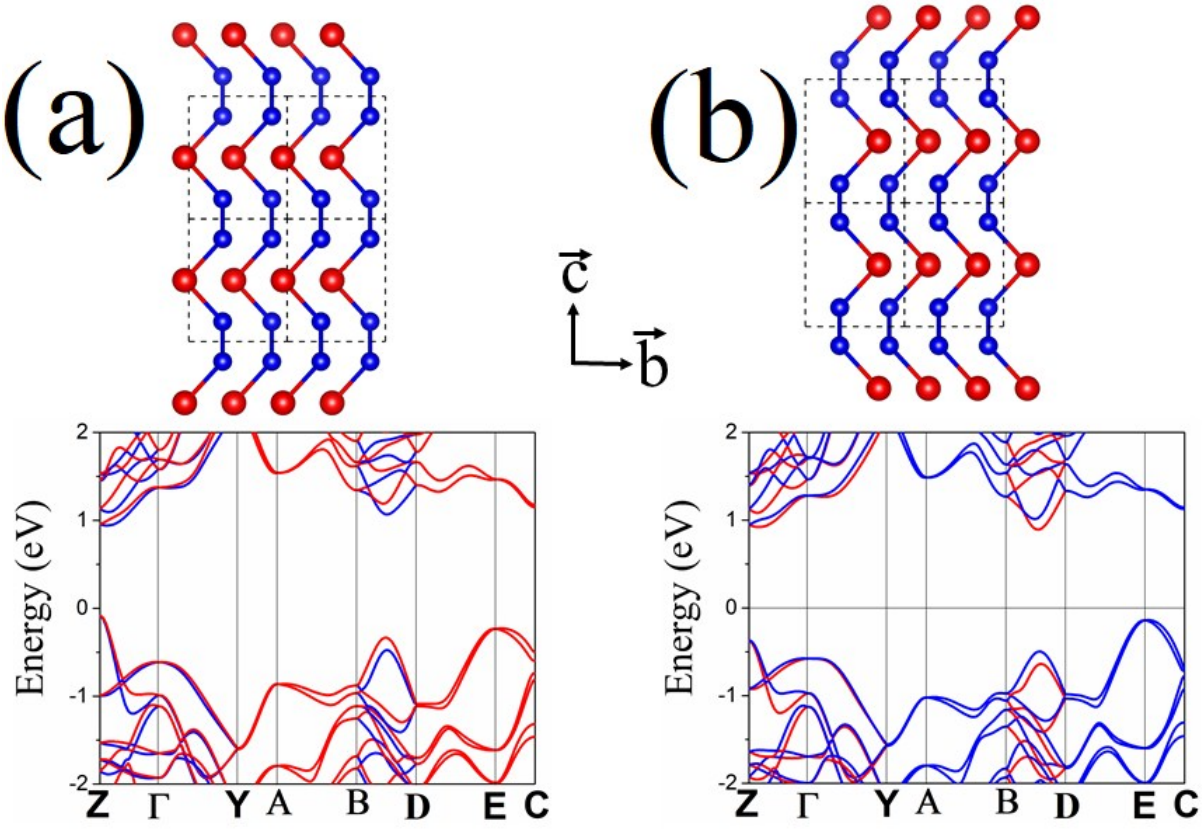


Figure S5. The chemical structure and MBJLDA +SOC band structure of bulk $TeSe_2$ in the M_H (a) and $M^L{}_H$ (b) phases. The red and blue lines in band structures represent spin up and down states, respectively.

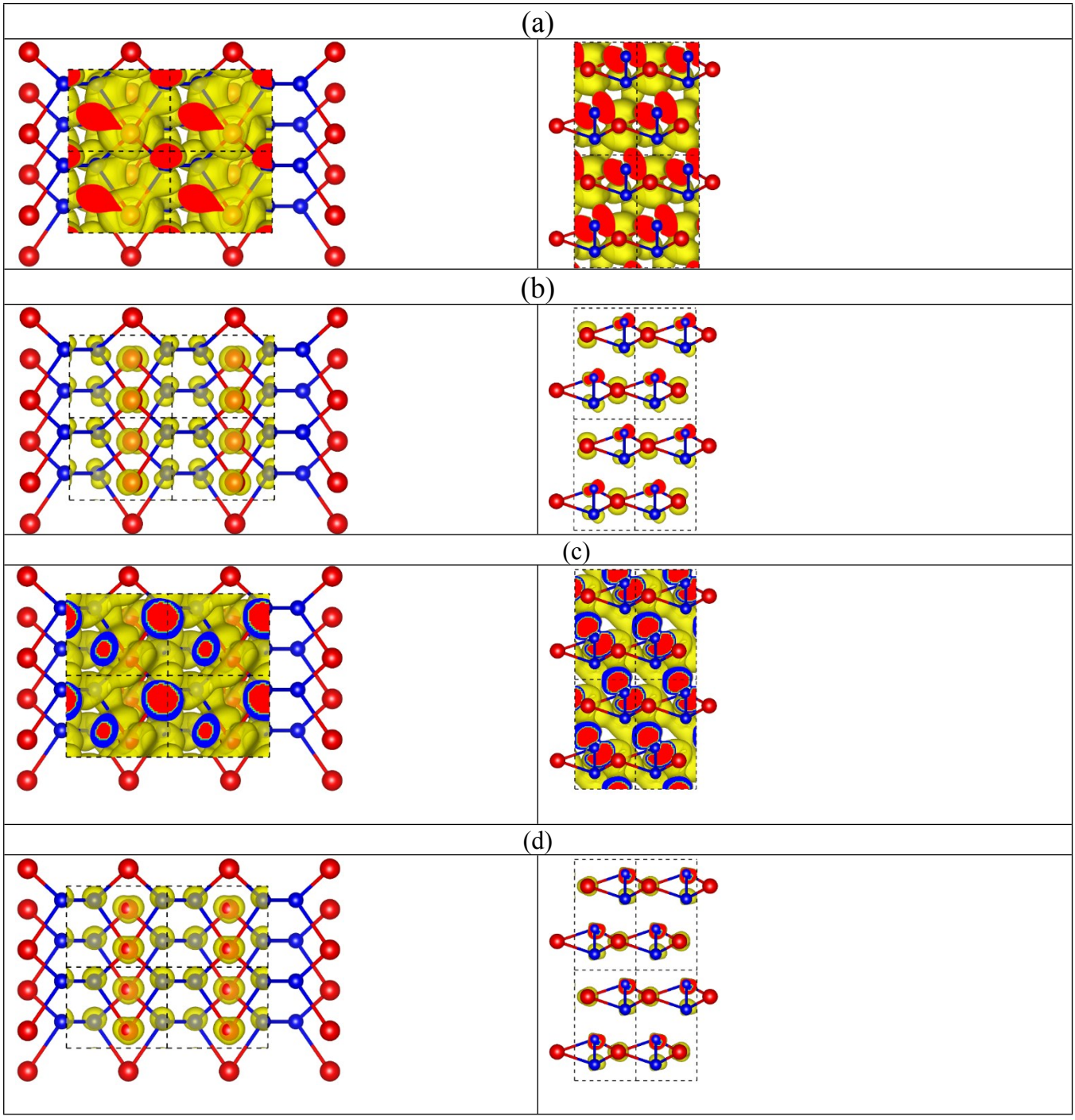


Figure S6. Two different views of the charge density plot of of the valence band in the $M_{\beta\alpha}$ at Γ' (Γ→Y) (a) and Z'' (Γ→Z) (b) points. Similar plots are also shown for the conduction band at Γ''' (Γ→Y) (c) and Z'''' (Γ→Z) (d) points. The charge density visualization is shown with isosurface of 0.0003 eÅ^{-3}. The red and blue balls represent Te and Se atoms, respectively.

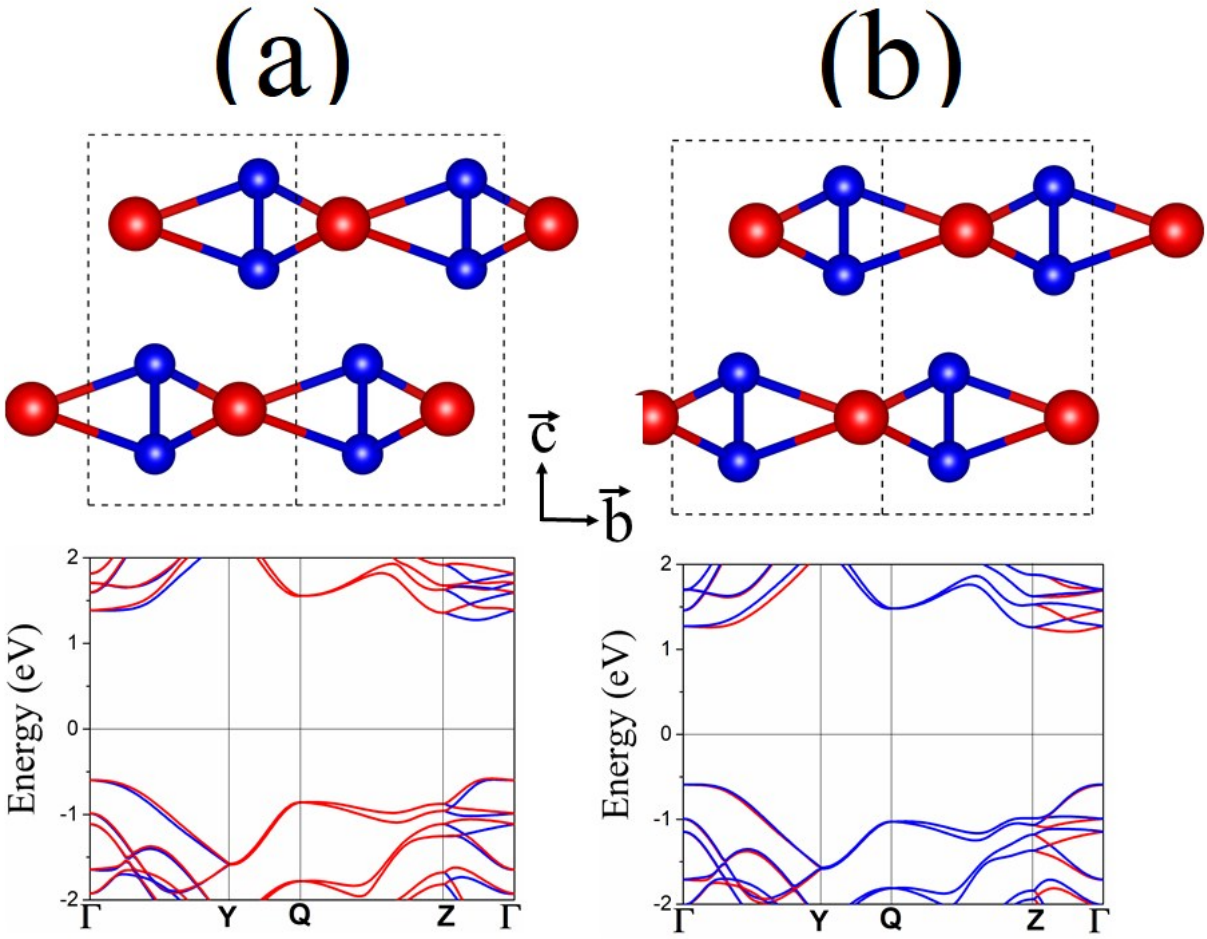


Figure S7. The chemical structure and MBJLDA +SOC band structure of bulk $TeSe_2$ in the $M_{\beta\alpha}$ (a) and $M^{L}_{\beta\alpha}$ (b) phases. The red and blue lines in band structures represent spin up and down states, respectively.