Supporting Information

Topological Insulators based on 2D Shape-persistent Organic Ligand Complexes

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Table S1 The energy differences between *cis*- and *trans*-structures.

Complex	$\Delta E = E_{cis} - E_{trans}$ (eV/unit cell)
Pd-$(NH_2)S$	1.28
Pt-$(NH_2)S$	1.44
Pd-$(NH_2)O$	2.50
Pt-$(NH_2)O$	2.40
Pd-(NH)S	0.03
Pt-(NH)S	0.19

Table S2 The lattice constant (a) and Pd/Pt-N distance (d) in each *trans*-complex.

Complex	a /Å	d / Å
trans-Pd-(NH$_2$)S	23.15	2.073
trans-Pt-(NH$_2$)S	23.14	2.063
trans-Pd-(NH$_2$)O	22.35	2.062
trans-Pt-(NH$_2$)O	22.37	2.051
trans-Pd-(NH)S	22.94	1.977
trans-Pt-(NH)S	22.95	1.968
trans-Pd-(NH)O	22.24	1.969
trans-Pt-(NH)O	22.27	1.954
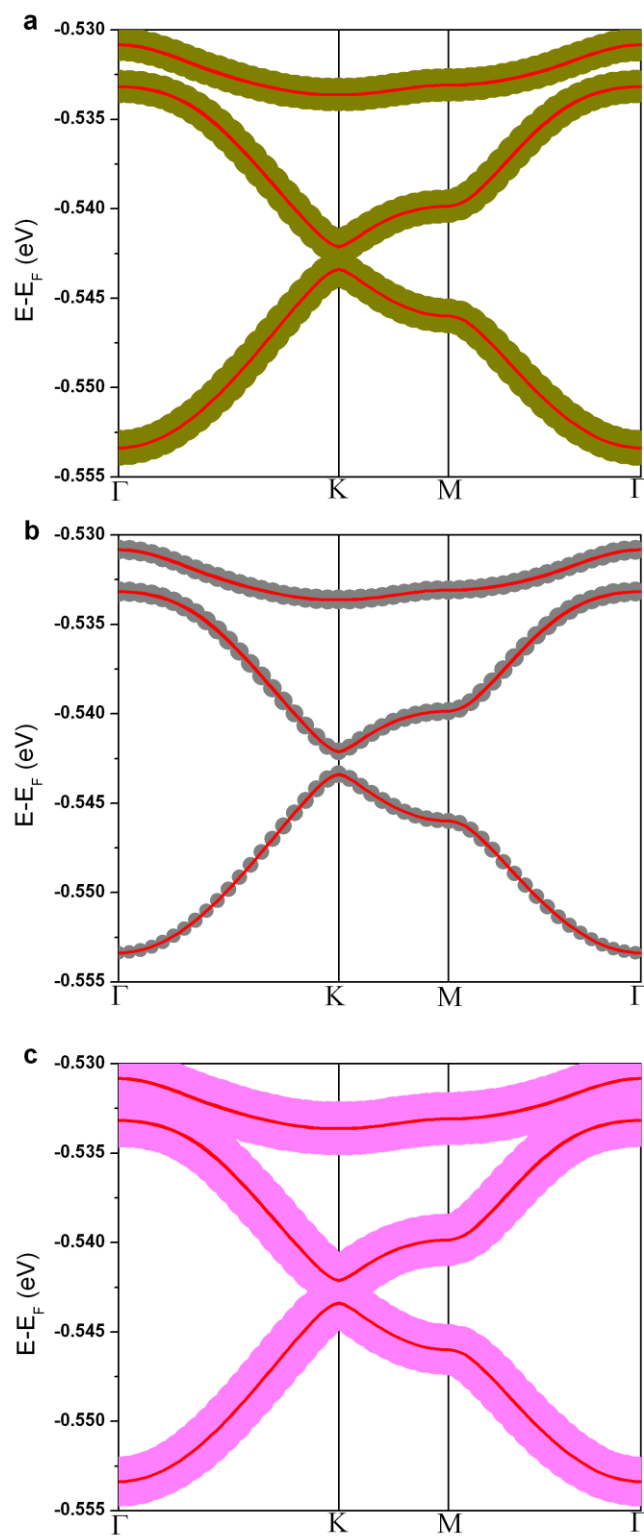
Fig. S1 (a) – (c) The occupancies of *p*-orbital components from S (yellow), C (grey) and the sum of them (pink) in three topmost kagome bands in 2D *trans*-Pd-(NH$_2$)S complex.
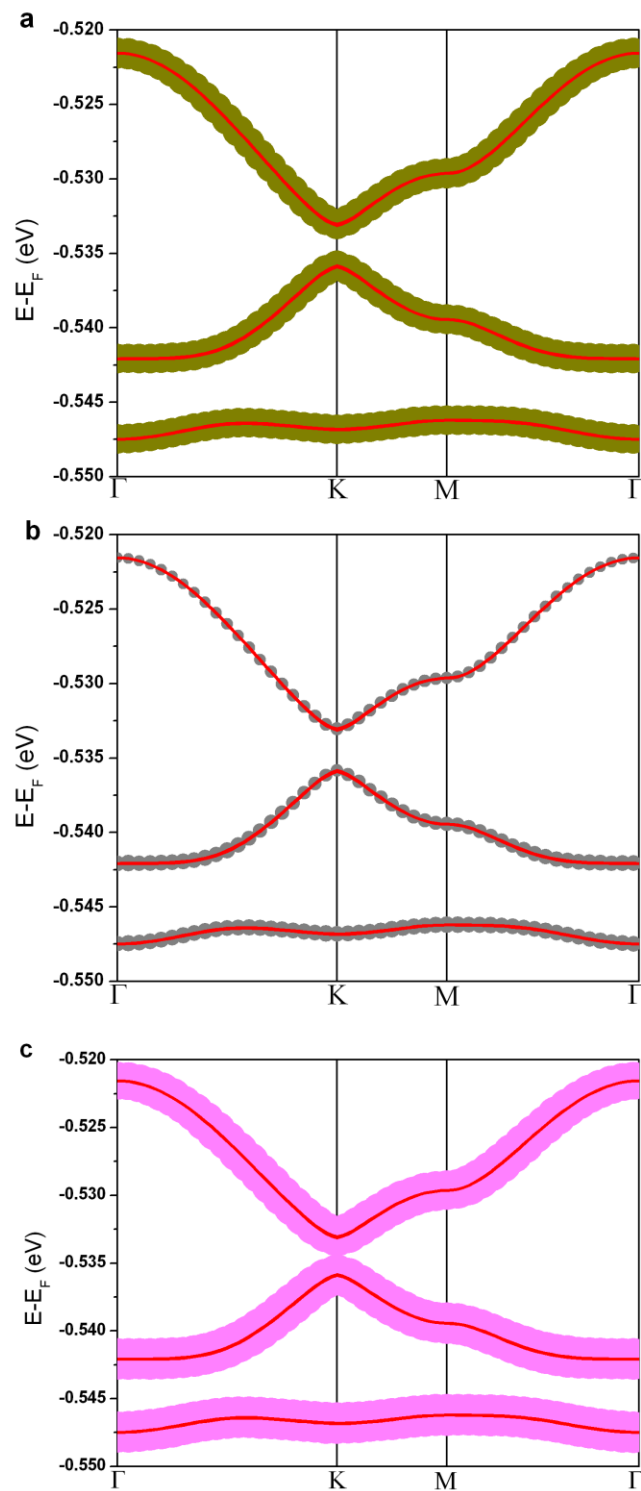
Fig. S2 (a) – (c) The occupancies of *p*-orbital components from S, C atoms and the sum of them in three topmost kagome bands in 2D *trans*-Pt-(NH$_2$)S complex.
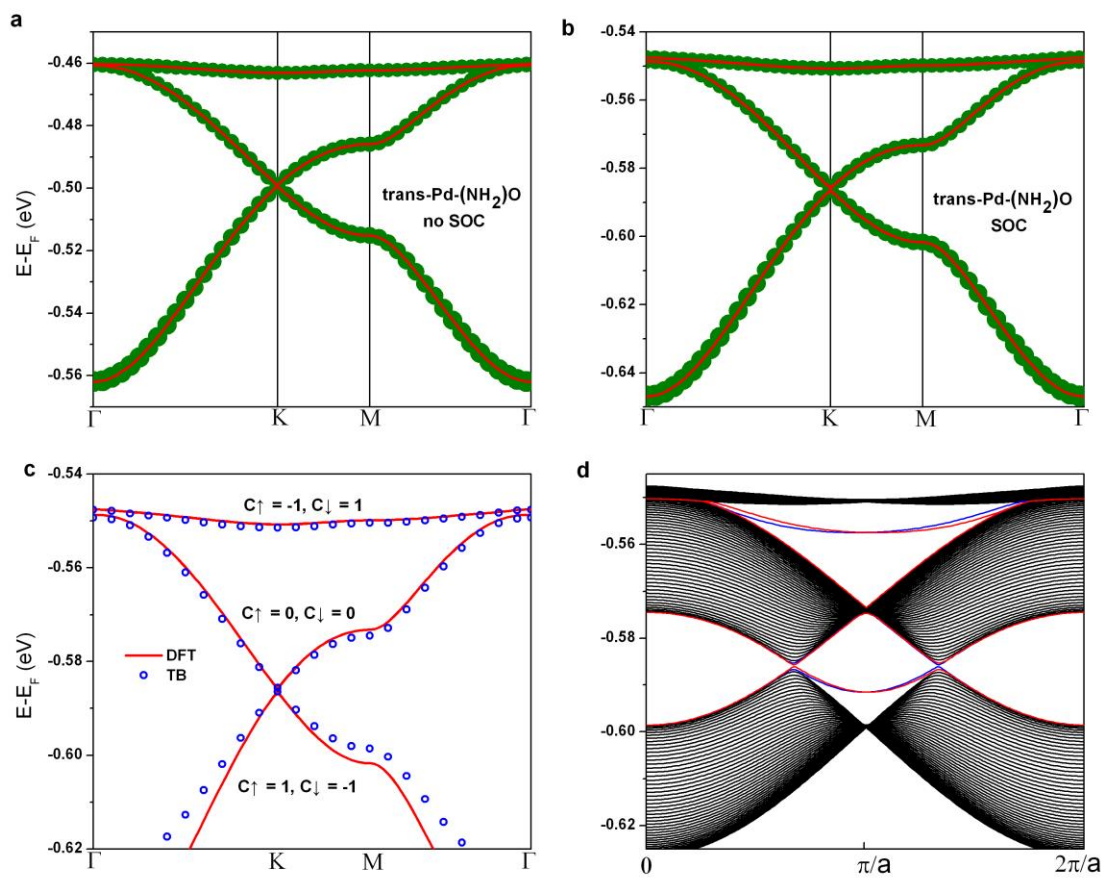
Fig. S3 DFT calculated band structures of *trans*-Pd-(NH$_2$)O (a) without and (b) with SOC consideration as well as *d*-orbital occupancies; (c) comparison between DFT and TB calculated band structures; (d) edge states for both up and down spins.
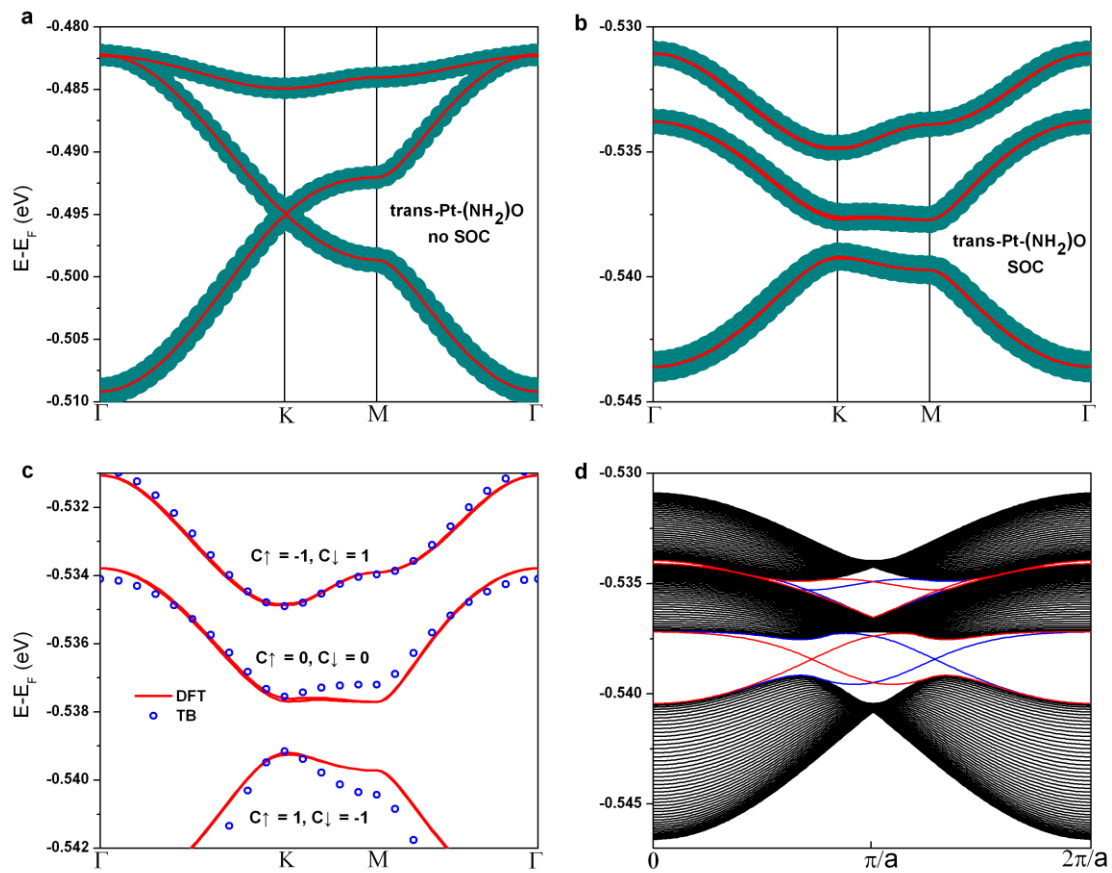
Fig. S4 DFT calculated band structures of *trans*-Pt-(NH$_2$)O (a) without and (b) with SOC consideration as well as *d*-orbital occupancies; (c) comparison between DFT and TB calculated band structures; (d) edge states for both up and down spins.
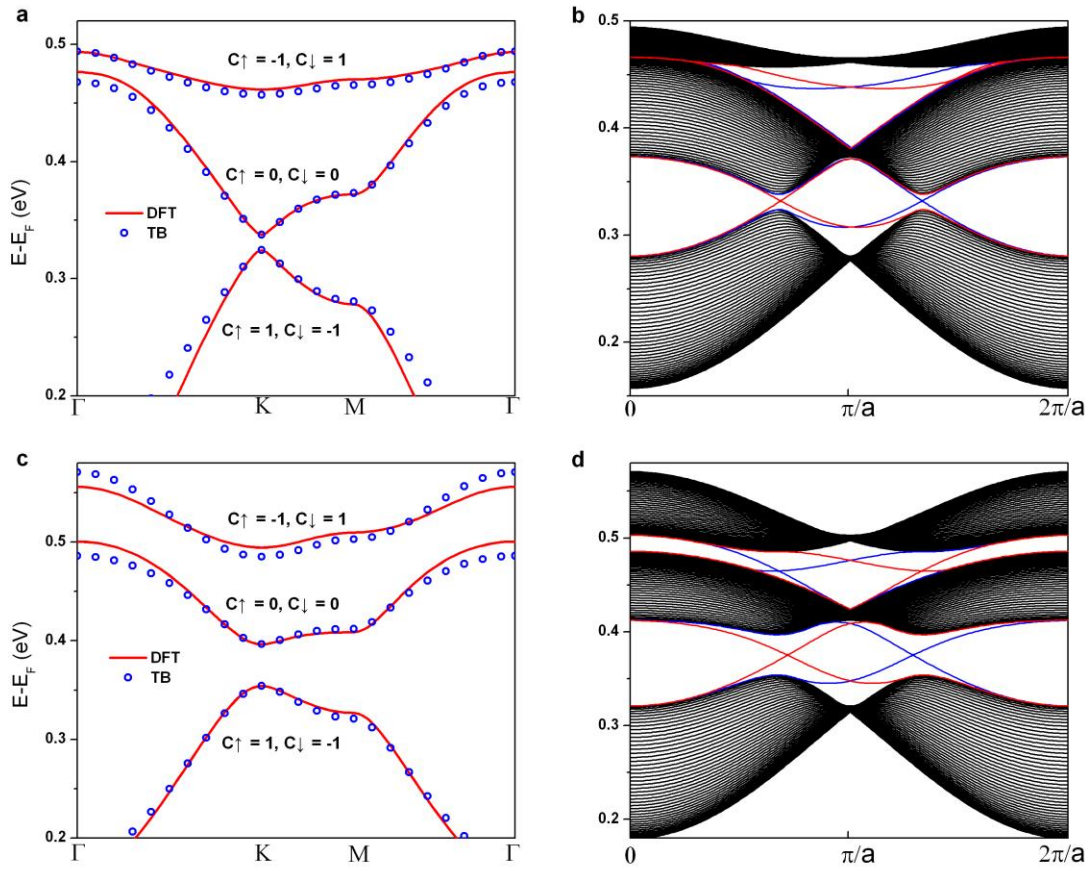
Fig. S5 (a) Comparison between DFT and TB calculated band structures with SOC considerations for *trans*-Pd-(NH)S; and (b) edge states for both up and down spins. The calculated Z_2 invariants are equal to 1 in both gaps. (c) and (d) are for *trans*-Pt-(NH)S.
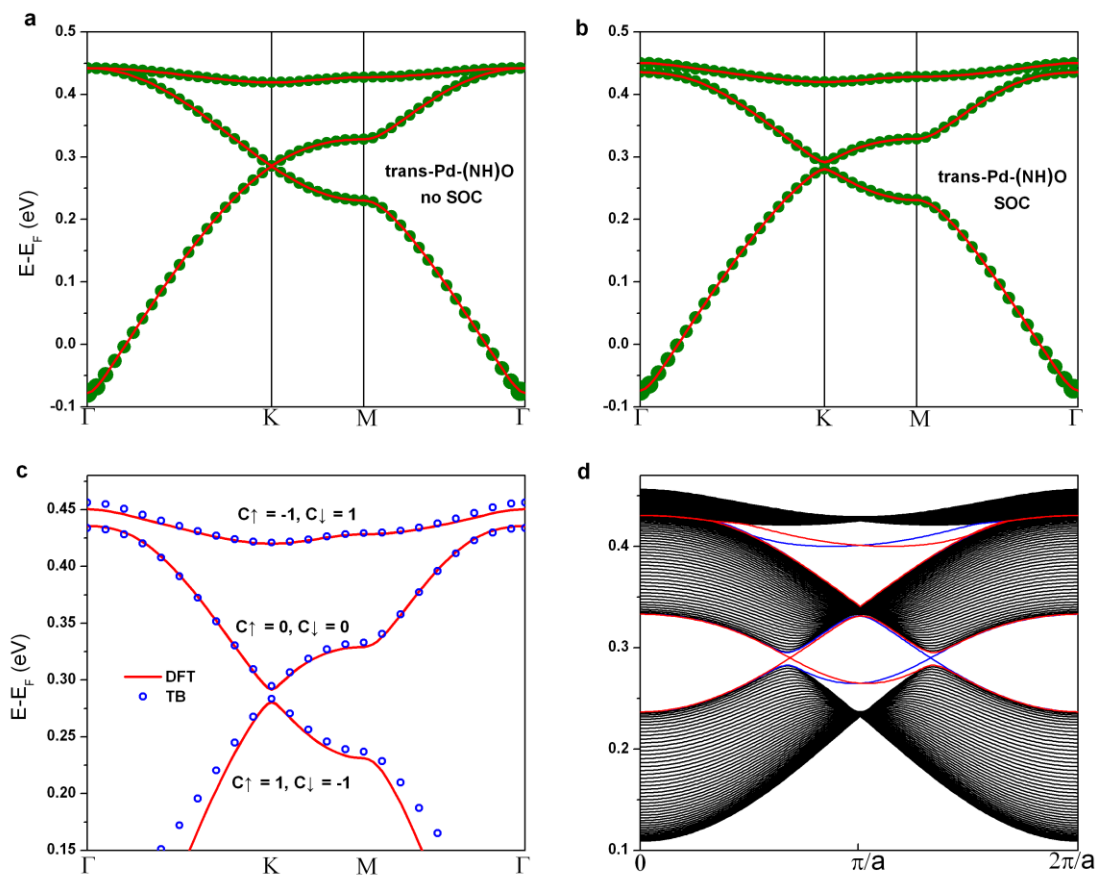
Fig. S6 (a) & (b) DFT calculated band structures of *trans*-Pd-(NH)O without and with SOC considerations; (c) comparison between DFT and TB calculated band structures; and (d) edge states for both spins. Z_2 invariants are calculated to 1 in both gaps.
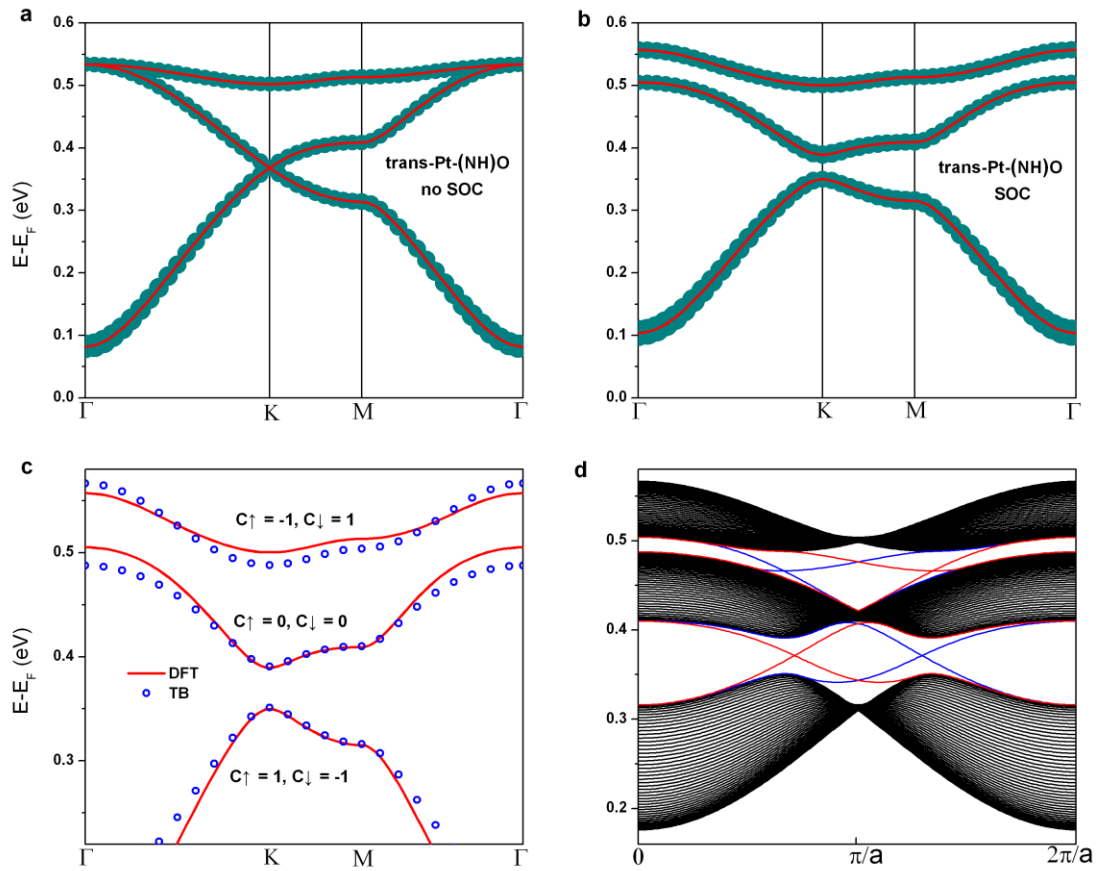
Fig. S7 (a) & (b) DFT calculated band structures of *trans*-Pt-(NH)O without and with SOC considerations; (c) comparison between DFT and TB calculated band structures; and (d) edge states for both spins. Z_2 invariants are calculated to be 1 in both gaps.
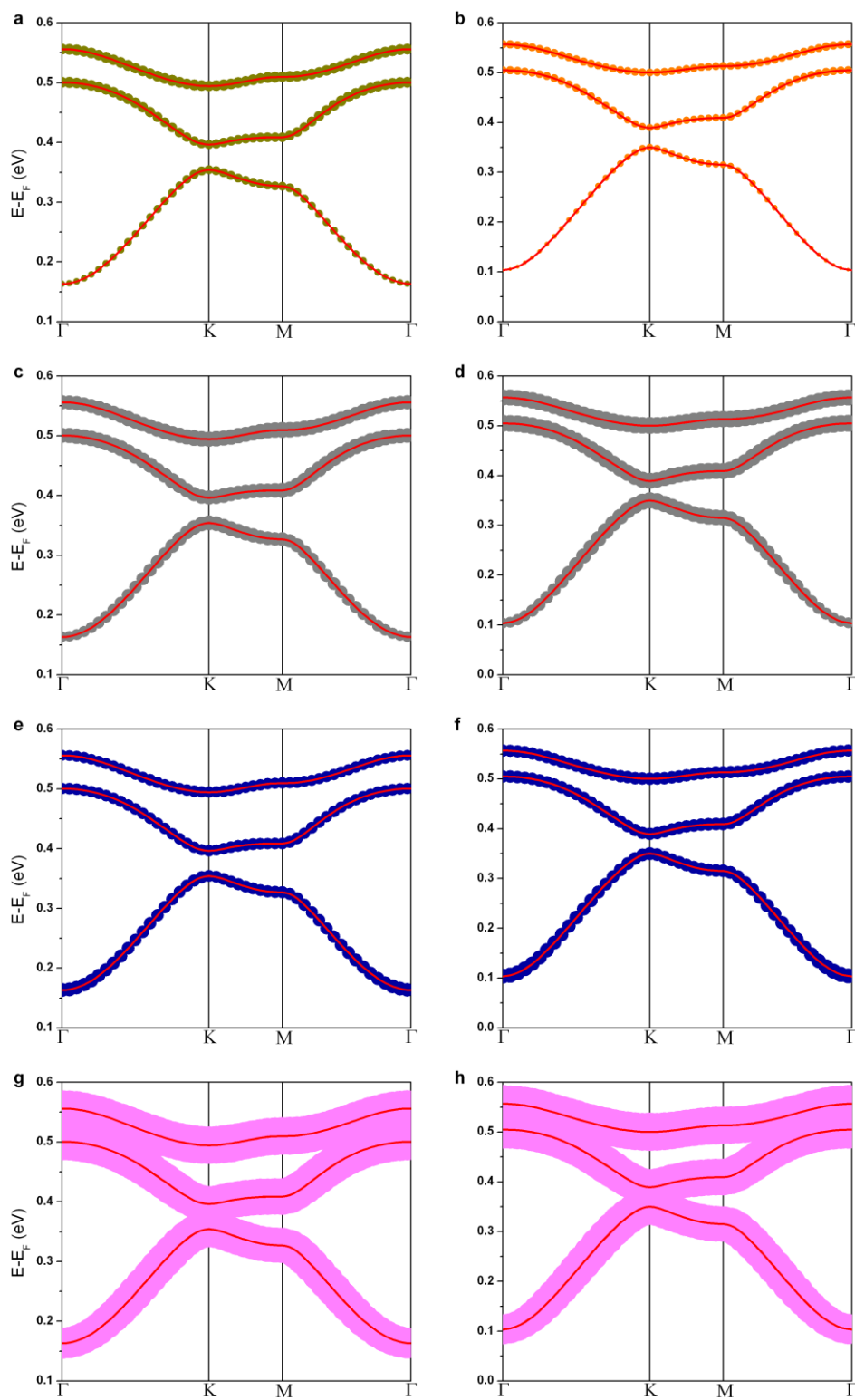
Fig. S8 *p*-orbital occupancies from S/O, C, N atoms and sum of them for *trans*-Pt-(NH)S (a, c, e, g) and for *trans*-Pt-(NH)O (b, d, f, h).
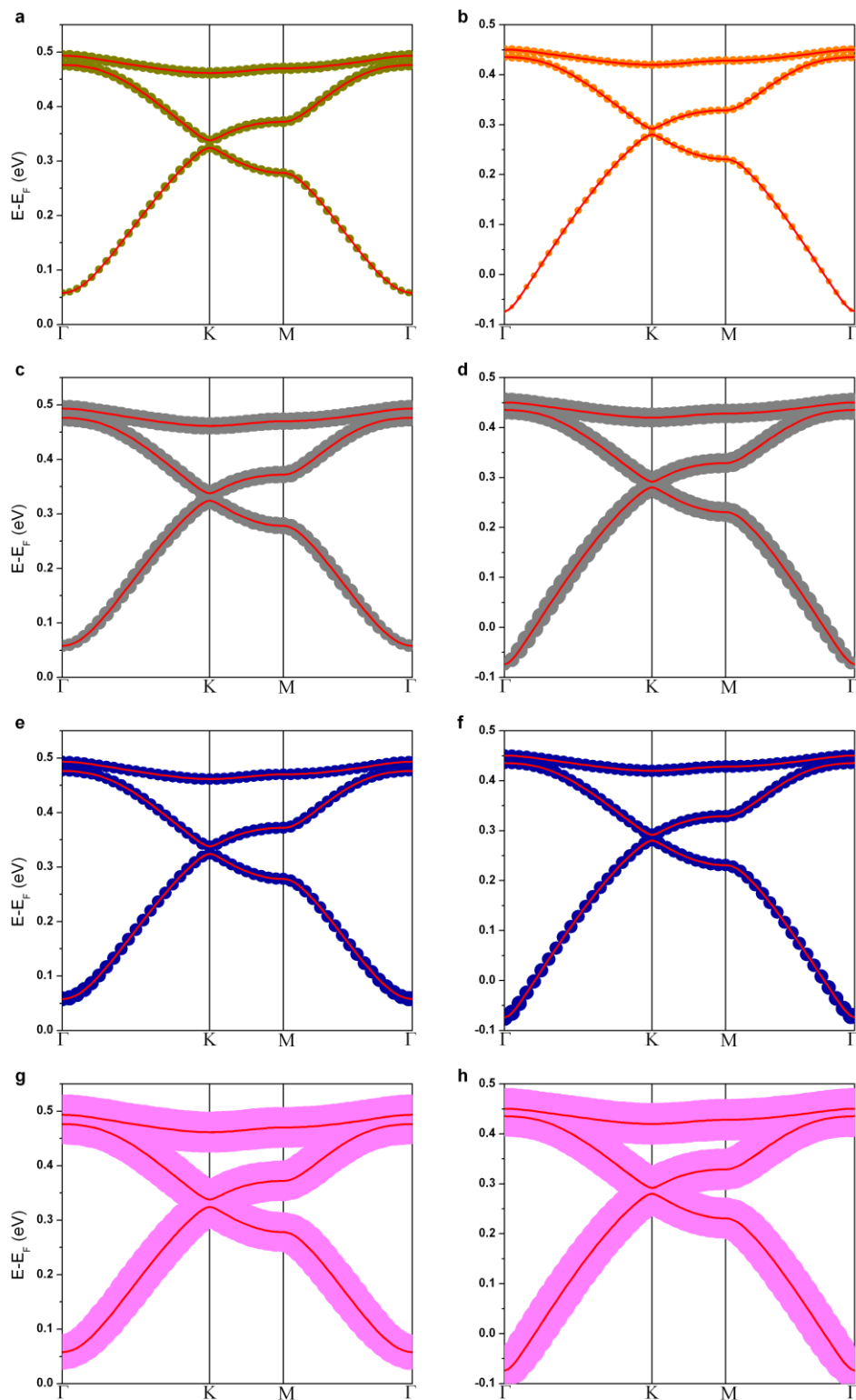
Fig. S9 *p*-orbital occupancies from S/O, C, N atoms and sum of them for *trans*-Pd-(NH)S (a, c, e, g) and *trans*-Pd-(NH)O (b, d, f, h) respectively.
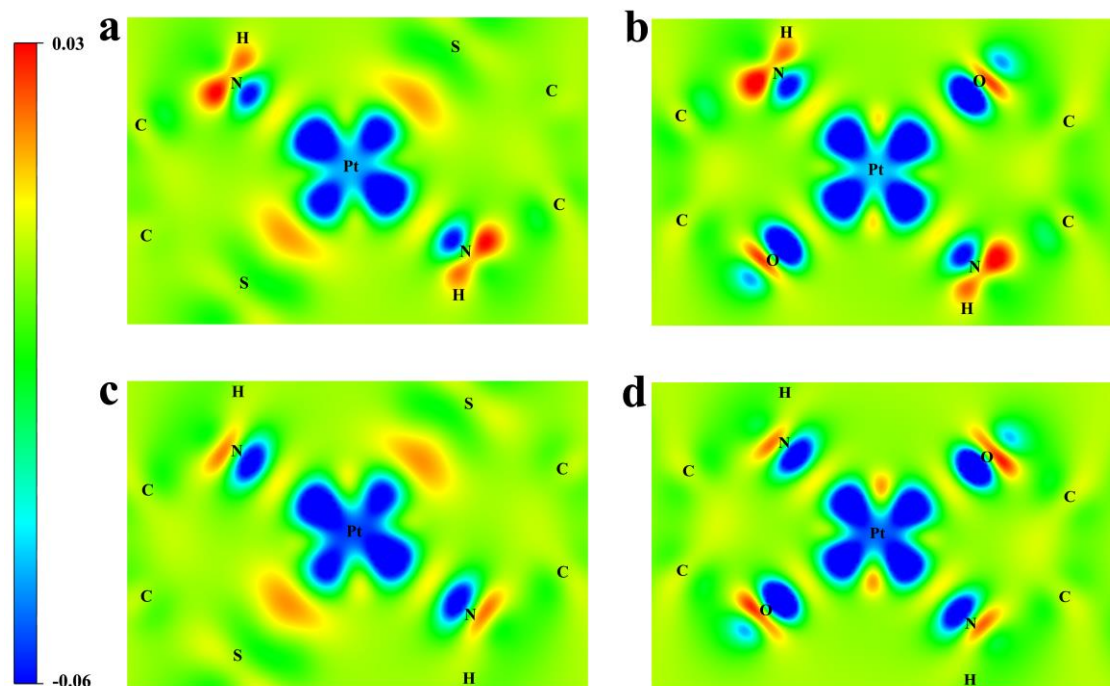
Fig. S10 Charge density difference of *trans*-structures: (a) Pt-(NH$_2$)S; (b) Pt-(NH$_2$)O; (c) Pt-(NH)S; and (d) Pt-(NH)O respectively. The unit of the scale is e/Å^3.
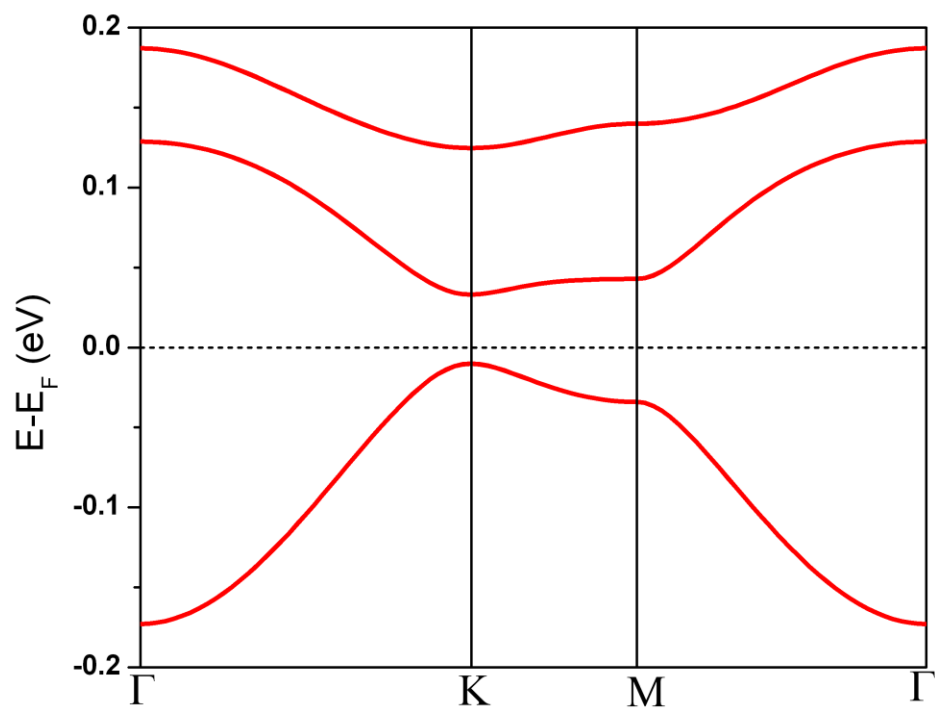
Fig. S11 DFT calculated band structures based on Jellium Model electron-doped (two electrons per unit cell) for *trans*-Pt-(NH)S complex with SOC consideration.