Supplementary Information for "Competition between Ta-Ta and Te-Te bonding leading to the commensurate charge density wave in $TaTe_4$"

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TABLE S-I. Comparison between the experimental coordinates (taken from [1]) and those calculated for the $TaTe_4$ modulated structure in its $2a\times2a\times3c$ phase.

		Experimental			Calculated		
Atom type	Wyckoff Position	x	y	z	x	y	z
Ta 1	8e	0.0000	0.0000	0.09652	0.0000	0.0000	0.09668
Ta 2	4a	0.0000	0.0000	0.25000	0.0000	0.000	0.25000
Ta 3	4c	0.0000	0.5000	0.41827	0.0000	0.5000	0.41828
Ta 4	4c	0.0000	0.5000	0.26351	0.0000	0.5000	0.26385
Ta 5	4c	0.0000	0.5000	0.07030	0.0000	0.5000	0.07005
Te 1	16g	0.0611	0.1579	-0.00300	0.0832	0.1653	-0.00176
Te 2	16g	0.5802	0.1655	0.00170	0.5911	0.1874	-0.00049
Te 3	16g	0.1656	0.0789	0.16860	0.1828	0.0933	0.16734
Te 4	16g	0.6665	0.5747	0.16970	0.6774	0.5796	0.16336
Te 5	16g	0.6687	0.0700	0.16330	0.6673	0.0827	0.16871
Te 6	16g	0.1561	0.5648	0.16750	0.1717	0.5817	0.16943

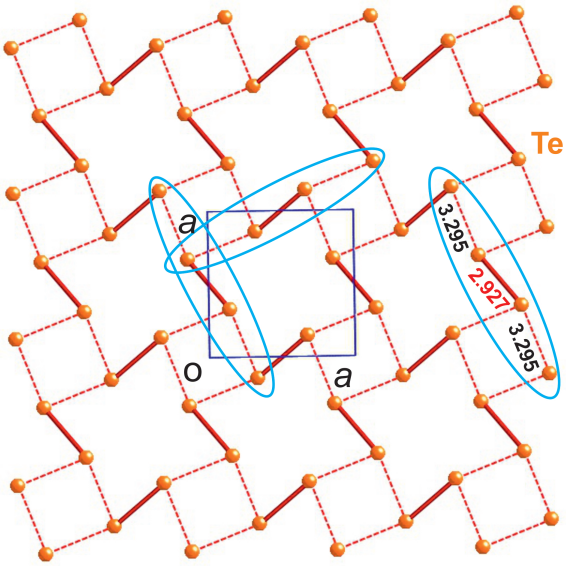

FIG. S1. View of one of the tellurium (aa) planes in the crystal structure of $TaTe_4$ showing in-plane Te...Te short contacts and Te-Te bonds. The distances refer to the average crystal structure [1].

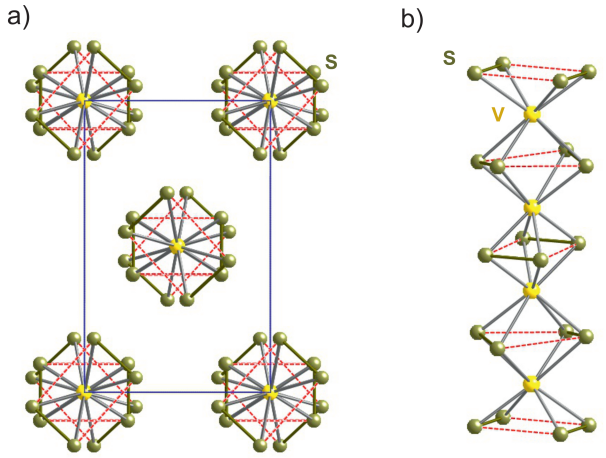

FIG. S2. (a) Top view of the VS_4 crystal structure. (b) Lateral view of a VS_4 chain showing the rectangular antiprismatic coordination of the V atoms and the structural dimerization (i.e. four V atoms per repeat unit). The full and dashed lines refer to the short and long S-S contacts in the rectangular S_4 units [2].

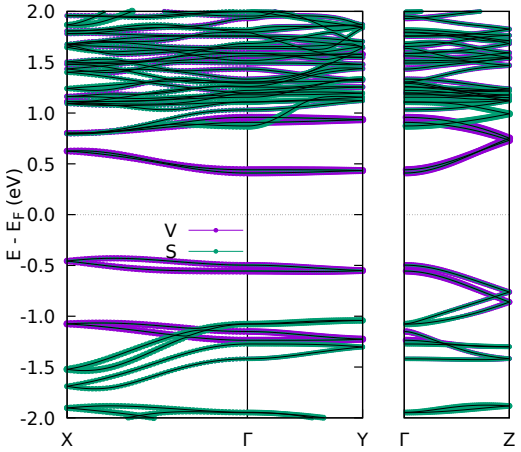

FIG. S3. Fatband structure of VS_4 where the green and purple full circles are associated with the S $3p$ and V $3d_{z^2}$ contributions.

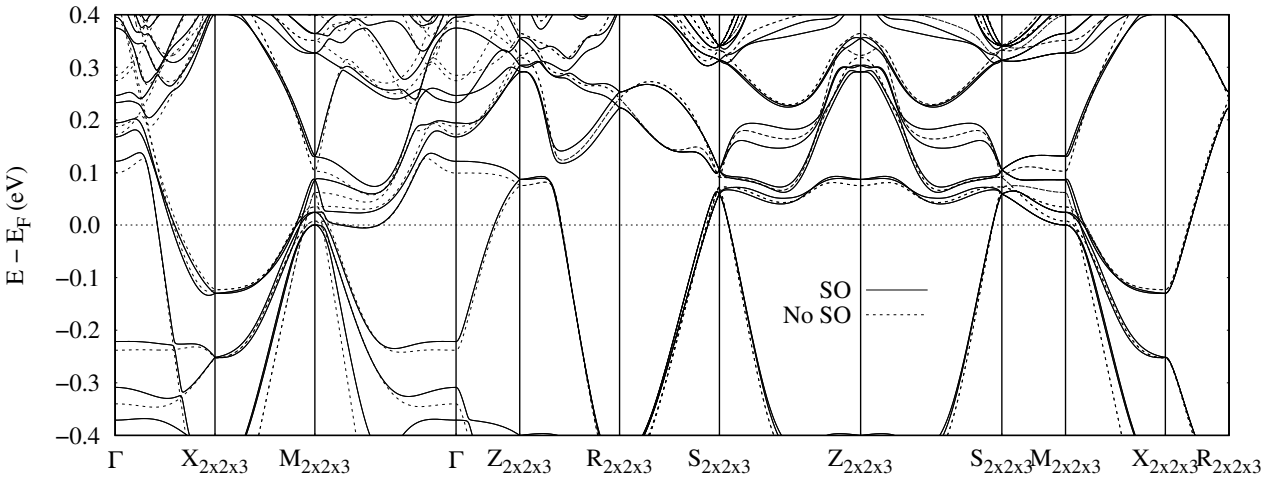

FIG. S4. Comparison between band structures with and without the inclusion of Spin-Orbit (SO) coupling in the $2a\times2a\times3c$ modulated $TaTe_4$ structure.

[1] K. D. Bronsema, S. van Smaalen, J. D. Boer, G. A. Wiegers, F. Jellinek, and J. Mahy, Acta Crystallogr. B **43**, 305–313 (1987).
[2] I. B. R. Allmann, A. Kutoglu, H. Roesch, and E. Hellner, Naturwissenschaften **51**, 263 (1964)