Supporting Information for

Pressure-induced superconductivity in topological semi-metal $TaM_2(M = As, Sb)$

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Structural properties

Table S1 listed the ground state structural parameters of topological semi-metal $TaM_2(M = As, Sb)$ which also include various experimental and theoretically simulated data. To determine the structural parameters listed in Table S2, both compounds are subjected to hydrostatic pressure from 0 to 40 GPa. The structural properties are significantly affected by the application of pressure. As pressure is increased, the lattice constants and unit cell volume decrease.

Table S1. Ground state structural parameters for topological semi-metal $TaM_2(M = As, Sb)$.

Materials	Pressure (GPa)	a (Å)	b (Å)	c (Å)	V (Å^3)	ΔE_f (eV)	Ta-M (M=As,Sb) (Å)	Remarks
$TaAs_2$	0	9.44	3.43	7.88	254.54	-41.94	2.72	[This work]
	0	9.37	3.39	7.77	--	--	--	Expt. [1]
	0	9.33	3.39	7.84	--	--	--	Expt. [2]
	0	9.44	3.42	7.84	--	--	--	Calc. [3]
	10	9.27	3.33	7.70	237.68	-41.93	2.66	[This work]
	20	9.15	3.26	7.58	225.84	-41.89	2.62	[This work]
	30	9.05	3.20	7.47	216.03	-41.83	2.59	[This work]
	40	8.97	3.14	7.39	208.29	-41.77	2.56	[This work]
$TaSb_2$	0	10.33	3.69	8.40	320.38	-38.21	2.92	[This work]
	0.5	10.21	3.64	8.28	--	--	--	Expt. [4]
	0	10.22	3.65	8.29	--	--	--	Expt. [5]
	0	10.36	3.70	8.39	--	--	--	Calc. [3]
	10	10.11	3.56	8.19	294.81	-38.18	2.85	[This work]
	20	9.96	3.46	8.04	277.24	-38.13	2.81	[This work]
	30	9.85	3.39	7.92	264.07	-38.05	2.76	[This work]
	40	9.76	3.32	7.82	253.51	-37.97	2.73	[This work]

Elastic properties

Elastic constants are crucial quantities because they describe the relationship between a solid's mechanical and dynamical properties. These constants are used to explain the connection between the phonon spectrum and the Debye temperature of crystals, and thus the mechanical stability of the solid itself. It is necessary to study the elastic characteristics of superconducting material because the elastic properties of any chemical are roughly connected to the long-wavelength phonon spectrum [6]. The estimated elastic constants of topological semi-metal $TaAs_2$ and $TaSb_2$ at various pressures are represented in Tables S2 and S3, respectively.

Table S2. The calculated values of elastic constants C_{ij} (in GPa) of topological semi-metal $TaAs_2$ at various applied pressures.

P	C_{11}	C_{12}	C_{13}	C_{15}	C_{22}	C_{23}	C_{25}	C_{33}	C_{35}	C_{44}	C_{46}	C_{55}	C_{66}
0	286.68	77.99	73.81	-17.79	220.84	54.56	18.63	253.94	-5.65	89.53	4.31	105.89	90.37
10	367.05	107.79	114.59	-24.99	285.21	90.19	28.29	344.29	-1.79	125.26	32.24	131.63	137.50
20	414.05	137.16	140.05	-40.97	331.56	89.24	26.24	406.29	-54.06	123.85	44.07	137.94	127.72
30	491.45	166.73	186.54	-45.36	386.09	144.79	20.53	471.46	1.82	157.39	33.69	145.99	111.57
40	541.69	197.56	220.49	-48.74	414.61	164.12	22.77	528.59	-13.16	146.67	20.18	165.93	142.23

Table S3. The calculated values of elastic constants C_{ij} (in GPa) of topological semi-metal $TaSb_2$ at various applied pressures.

P	C_{11}	C_{12}	C_{13}	C_{15}	C_{22}	C_{23}	C_{25}	C_{33}	C_{35}	C_{44}	C_{46}	C_{55}	C_{66}
0	220.59	68.86	53.79	-19.99	148.27	43.25	14.13	211.89	3.13	75.97	21.84	83.22	74.68
10	291.17	103.55	83.86	-31.95	220.47	80.00	8.28	312.69	-3.45	112.89	23.31	94.28	120.46
20	361.79	130.37	121.99	-40.01	255.41	112.94	14.95	370.89	3.52	126.86	37.34	118.67	118.21
30	455.75	170.17	148.70	-48.11	296.18	120.60	19.24	400.85	-2.41	123.34	43.17	139.92	139.77
40	493.36	201.41	181.47	-55.71	348.86	171.91	18.26	476.65	-3.53	154.97	50.28	150.66	140.95

Mechanical Properties

Material's mechanical properties include the Young's modulus (*E*), shear modulus (*G*), bulk modulus (*B*), Poisson's ratio (*ν*), and anisotropic factor (*A*) are tabulated in Table S6 and S7. Table S6 and S7 show that all *B/G* values for $TaM_2 (M = As, Sb)$ materials are higher than the critical value 1.75, indicating that these materials are ductile.

Table S4. The calculated bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Pugh's ratio B/G and Poisson's ratio ν of topological semi-metal $TaAs_2$.

P (GPa)	B_V	B_R	B	G_V	G_R	G	E	B/G	ν
0	130.46	128.12	129.29	94.16	91.79	92.98	225.00	1.39	0.21
10	180.19	177.04	178.61	124.48	117.62	121.05	296.23	1.48	0.22
20	209.42	203.06	206.24	130.27	116.92	123.59	309.04	1.67	0.25
30	260.57	255.82	258.19	139.72	130.39	135.05	345.01	1.91	0.28
40	294.36	287.00	290.68	151.15	145.17	148.16	379.93	1.96	0.28

Table S5. The calculated bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Pugh's ratio B/G and Poisson's ratio ν of topological semi-metal $TaSb_2$.

P (GPa)	B_V	B_R	B	G_V	G_R	G	E	B/G	ν
0	101.39	97.85	99.62	74.43	67.87	71.15	172.41	1.40	0.21
10	151.02	147.96	149.49	102.65	95.02	98.84	242.97	1.51	0.23
20	190.97	185.50	188.23	114.27	103.59	108.93	273.95	1.73	0.26
30	225.75	216.19	220.97	128.16	114.83	121.50	308.04	1.82	0.27
40	269.83	262.90	266.36	140.25	125.18	132.72	341.44	2.01	0.29

Table S6 shows the variation of *B, G, E, B/G,* ν with other experimental and theoretically simulated work of different topological semi-metals.

Table S6. The ground state bulk modulus B (GPa), shear modulus G (GPa), Young's modulus E (GPa), Pugh's ratio B/G and Poisson's ratio ν of different topological semi-metals.

Materials	B_V	B_R	B	G_V	G_R	G	E	B/G	ν	Remarks
$TaAs_2$	130.46	128.12	129.29	94.16	91.79	92.98	225.00	1.39	0.21	[This work]
$TaSb_2$	101.39	97.85	99.62	74.43	67.87	71.15	172.41	1.40	0.21	[This work]
$NiTe_2$	--	--	70.12	--	--	28.75	50.95	2.44	0.32	Calc. [10]
$MoTe_2$	60.35	48.31	54.33	35.97	43.02	39.49	95.37	1.38	0.207	Calc. [8]
WTe_2	58.26	38.91	48.59	44.12	34.52	39.32	92.89	1.24	0.18	Calc. [9]

Table S8 and Table S9 show the the maximum and minimum value of *E, β, G,* and *ν* for both compounds. This value increases with applied pressure but the *β* value decreases for both materials.

Table S7. The minimum and maximum limits of E (GPa), β (TP^{-1}), G (GPa), and ν of the topological semi-metal $TaAs_2$.

P (GPa)	E			β			G			ν		
	E_{min}	E_{max}	A_E	β_{min}	β_{max}	A_β	G_{min}	G_{max}	A_G	ν_{min}	ν_{max}	A_ν
0	188.78	287.59	1.52	1.92	3.19	1.67	74.61	110.14	1.48	0.07	0.36	4.83
10	228.95	367.99	1.61	1.41	2.42	1.72	89.62	164.20	1.83	0.08	0.40	4.87
20	219.49	449.85	2.05	1.08	1.99	1.86	81.67	174.55	2.14	0.02	0.50	24.37
30	260.24	462.28	1.78	1.00	1.70	1.69	93.73	175.22	1.87	0.12	0.49	4.11
40	306.01	511.09	1.67	0.84	1.59	1.89	115.34	181.97	1.58	0.11	0.43	3.81

Table S8. The minimum and maximum limits of E (GPa), β (TP^{-1}), G (GPa), and ν of the topological semi-metal $TaSb_2$.

P (GPa)	E			β			G			ν		
	E_{min}	E_{max}	A_E	β_{min}	β_{max}	A_β	G_{min}	G_{max}	A_G	ν_{min}	ν_{max}	A_ν
0	118.51	225.18	1.90	2.17	4.83	2.22	46.94	97.18	2.07	0.04	0.45	10.74
10	171.09	283.09	1.66	1.69	2.93	1.74	62.62	140.29	2.24	0.00	0.43	467.90
20	188.13	353.76	1.88	1.34	2.57	1.92	70.74	160.13	2.26	0.05	0.49	10.47
30	207.69	423.03	2.04	0.89	2.26	2.55	77.92	175.50	2.25	0.05	0.56	10.63
40	233.15	460.75	1.98	0.88	1.79	2.03	84.72	198.72	2.35	0.06	0.55	8.83

Electronic properties

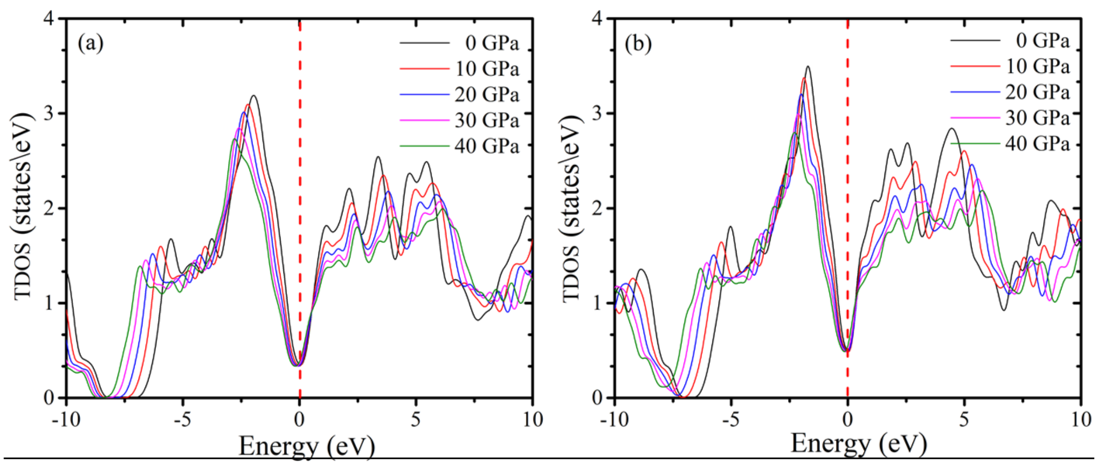

Figure S1. Simulated (a) TDOS of the $TaAs_2$ compound and (b) TDOS of the $TaSb_2$ compound at pressures at 0, 10, 20, 30, and 40 GPa.

Thermodynamic properties

Table S9. The calculated Density ρ (Kg/m^3), Transverse velocity v_t (m/s), Longitudinal velocity v_l (m/s), mean sound velocity v_m (m/s), and Debye Temperature $\Theta_D(K)$ of topological semi-metal Ta^{M_2} (M=As, Sb)

Pressure (GPa)	Ta^{As_2}					Ta^{Sb_2}				
	ρ	v_t	v_l	v_m	θ_D	ρ	v_t	v_l	v_m	θ_D
0	8395.78	5492.32	3327.85	3677.85	395.98	8612.24	4752.11	2874.28	3177.14	316.82
10	8991.34	6149.41	3669.19	4061.20	447.36	9359.21	5482.10	3249.73	3599.16	368.99
20	9462.73	6261.73	3613.96	4012.30	449.56	9952.35	5788.49	3308.35	3676.11	384.68
30	9892.43	6655.99	3694.84	4115.40	467.99	10448.70	6054.12	3410.02	3793.72	403.48
40	10260.03	6898.21	3800.07	4235.13	487.50	10883.95	6382.13	3492.01	3893.82	419.80

Table S10. The ground state Density ρ (g/cm^3), Transverse velocity v_t (m/s), Longitudinal velocity v_l (m/s), mean sound velocity v_m (m/s), and Debye Temperature $\Theta_D(K)$ of different topological semi-metals.

Materials	ρ (gcm^{-3})	v_t (ms^{-1})	v_l (ms^{-1})	v_m (ms^{-1})	θ_D (K)	Remarks
$TaAs_2$	8.39	5492.3	3327.8	3677.9	395.98	[This work]
$TaSb_2$	8.61	4752.1	2874.3	3177.1	316.82	[This work]
$MoTe_2$	8.05	3644.7	2214.4	2446.6	252.06	Calc. [8]
WTe_2	9.86	3200.0	1996.5	2199.8	225.07	Calc. [9]

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