

## Transport properties of $\text{MoS}_2/\text{V}_7(\text{Bz})_8$ and graphene/ $\text{V}_7(\text{Bz})_8$ vdW junctions tuned by bias and gate voltages

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Table S1 lists the cartesian coordinates of  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$  vdW junction.

Table S2 lists the cartesian coordinates of graphene/ $\text{V}_7(\text{Bz})_8$  vdW junction.

Figure S1 corresponds to Figure 3. It gives the conductance for Channel S-D, Channel S-G, Channel D-G, and Channel G-G as a function of  $V_G$  at fixed values of  $V_S=0.0$ , 0.2, or 0.4 V of the four-terminal  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$  and graphene/ $\text{V}_7(\text{Bz})_8$  devices. (a) and (b) are for the  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$  and graphene/ $\text{V}_7(\text{Bz})_8$  devices, respectively. Here, the vertical-axis scales are adapted to their content.

Additional result:

Table S1 Cartesian coordinates of the MoS<sub>2</sub>/V<sub>7</sub>(Bz)<sub>8</sub> vdW junction

Atom	X	Y	Z
Au	50.57634	14.69631	21.84536
Au	50.57634	18.77457	21.84536
Au	50.57634	16.73544	19.80627
Au	50.57634	16.73544	23.8845
Au	5.097738	14.69631	21.84536
Au	5.097738	18.77457	21.84536
Au	5.097738	16.73544	19.80627
Au	5.097738	16.73544	23.8845
Au	48.53714	16.73544	21.84536
Au	48.53714	14.69631	19.80627
Au	48.53714	14.69631	23.8845
Au	48.53714	18.77457	19.80627
Au	48.53714	18.77457	23.8845
Au	7.136862	16.73544	21.84536
Au	7.136862	14.69631	19.80627
Au	7.136862	14.69631	23.8845
Au	7.136862	18.77457	19.80627
Au	7.136862	18.77457	23.8845
H	16.73279	15.36912	24.19692
H	23.08426	15.36912	24.19692
H	29.43578	15.36912	24.19692
H	35.78725	15.36912	24.19692
C	16.71586	15.98751	23.17738
C	23.06907	15.98751	23.17738
C	29.42059	15.98751	23.17738
C	35.77206	15.98751	23.17738
C	16.71586	17.52672	23.17344
C	23.06153	17.52672	23.17344
C	29.413	17.52672	23.17344
C	35.76451	17.52672	23.17344
H	16.71412	18.14322	24.1862
H	23.06559	18.14322	24.1862
H	29.41711	18.14322	24.1862
H	35.76858	18.14322	24.1862
C	16.74749	18.27246	21.83459
C	23.09896	18.27246	21.83459
C	29.45048	18.27246	21.83459
C	35.80195	18.27246	21.83459
H	16.72558	19.4574	21.82427
H	23.0771	19.4574	21.82427

H	29.42862	19.4574	21.82427
H	35.78014	19.4574	21.82427
C	16.71127	17.49921	20.51
C	23.06274	17.49921	20.51
C	29.41425	17.49921	20.51
C	35.76572	17.49921	20.51
H	16.71746	18.09828	19.48697
H	23.06893	18.09828	19.48697
H	29.42045	18.09828	19.48697
H	35.77191	18.09828	19.48697
C	16.71949	15.95889	20.53999
C	23.07101	15.95889	20.53999
C	29.42247	15.95889	20.53999
C	35.77399	15.95889	20.53999
H	16.73095	15.31971	19.53238
H	23.08247	15.31971	19.53238
H	29.43399	15.31971	19.53238
H	35.78546	15.31971	19.53238
C	16.76969	15.20298	21.86843
C	23.12116	15.20298	21.86843
C	29.47268	15.20298	21.86843
C	35.82415	15.20298	21.86843
V	18.33068	16.73544	21.84536
V	24.68215	16.73544	21.84536
V	31.03366	16.73544	21.84536
V	37.38514	16.73544	21.84536
C	19.9364	15.20112	21.86485
C	26.28792	15.20112	21.86485
C	32.63944	15.20112	21.86485
C	38.99096	15.20112	21.86485
C	19.91885	18.27831	21.83741
C	26.27032	18.27831	21.83741
C	32.62188	18.27831	21.83741
C	38.9734	18.27831	21.83741
C	19.89317	17.52801	23.17755
C	26.24464	17.52801	23.17755
C	32.59616	17.52801	23.17755
C	38.94767	17.52801	23.17755
C	19.89505	17.50581	20.5083
C	26.24657	17.50581	20.5083
C	32.59804	17.50581	20.5083
C	38.94956	17.50581	20.5083
C	19.89863	15.98493	23.17903
C	26.25015	15.98493	23.17903

C	32.60172	15.98493	23.17903
C	38.95319	15.98493	23.17903
C	19.89844	15.96108	20.53396
C	26.24991	15.96108	20.53396
C	32.60143	15.96108	20.53396
C	38.95299	15.96108	20.53396
H	19.89486	18.14466	24.18973
H	26.24633	18.14466	24.18973
H	32.59785	18.14466	24.18973
H	38.94937	18.14466	24.18973
H	19.89796	18.10968	19.48871
H	26.24947	18.10968	19.48871
H	32.60094	18.10968	19.48871
H	38.95246	18.10968	19.48871
H	19.91575	15.36627	24.19768
H	26.26727	15.36627	24.19768
H	32.61874	15.36627	24.19768
H	38.97026	15.36627	24.19768
H	19.91474	15.32559	19.52487
H	26.26621	15.32559	19.52487
H	32.61772	15.32559	19.52487
H	38.96919	15.32559	19.52487
H	19.90705	19.46361	21.8299
H	26.25852	19.46361	21.8299
H	32.61004	19.46361	21.8299
H	38.9615	19.46361	21.8299
V	21.48047	16.73469	21.84536
V	27.83198	16.73469	21.84536
V	34.1835	16.73469	21.84536
H	35.82415	14.11296	21.86843
H	38.99096	14.11113	21.86485
H	19.9364	14.11113	21.86485
H	16.76969	14.11296	21.86843
Au	13.25428	14.69631	21.84536
Au	13.25428	18.77457	21.84536
Au	9.175986	14.69631	21.84536
Au	9.175986	18.77457	21.84536
Au	15.29338	16.73544	21.84536
Au	11.21509	16.73544	21.84536
Au	15.29338	14.69631	19.80627
Au	15.29338	14.69631	23.8845
Au	15.29338	18.77457	19.80627
Au	15.29338	18.77457	23.8845
Au	11.21509	14.69631	19.80627

Au	11.21509	14.69631	23.8845
Au	11.21509	18.77457	19.80627
Au	11.21509	18.77457	23.8845
Au	13.25428	16.73544	19.80627
Au	13.25428	16.73544	23.8845
Au	9.175986	16.73544	19.80627
Au	9.175986	16.73544	23.8845
Au	42.41984	14.69631	21.84536
Au	42.41984	18.77457	21.84536
Au	46.49804	14.69631	21.84536
Au	46.49804	18.77457	21.84536
Au	40.38065	16.73544	21.84536
Au	44.45894	16.73544	21.84536
Au	40.38065	14.69631	19.80627
Au	40.38065	14.69631	23.8845
Au	40.38065	18.77457	19.80627
Au	40.38065	18.77457	23.8845
Au	44.45894	14.69631	19.80627
Au	44.45894	14.69631	23.8845
Au	44.45894	18.77457	19.80627
Au	44.45894	18.77457	23.8845
Au	42.41984	16.73544	19.80627
Au	42.41984	16.73544	23.8845
Au	46.49804	16.73544	19.80627
Au	46.49804	16.73544	23.8845
H	23.0771	14.11056	21.82427
H	29.42862	14.11185	21.82427
H	26.25852	14.11677	21.8299
H	32.61004	14.11272	21.8299
Mo	27.82004	10.28949	15.46532
Mo	27.82004	10.28949	26.41323
Mo	27.81854	10.24218	20.94274
Mo	27.81854	10.24218	31.89065
Mo	24.64302	10.28934	15.46402
Mo	24.64302	10.28934	26.41194
Mo	30.99454	10.28934	15.46402
Mo	30.99454	10.28934	26.41194
Mo	24.63122	10.24314	20.94144
Mo	24.63122	10.24314	31.8894
Mo	30.98269	10.24314	20.94144
Mo	30.98269	10.24314	31.8894
S	27.81694	8.57439	19.09758
S	27.81694	8.57439	30.04545
S	27.81786	8.60058	13.62244

S	27.81786	8.60058	24.57035
S	24.64331	8.5743	19.09749
S	24.64331	8.5743	30.04532
S	30.99483	8.5743	19.09749
S	30.99483	8.5743	30.04532
S	24.6422	8.60025	13.62163
S	24.6422	8.60025	24.56955
S	30.99372	8.60025	13.62163
S	30.99372	8.60025	24.56955
S	27.81748	11.9526	19.09923
S	27.81748	11.9526	30.04719
S	27.81593	11.97789	13.62825
S	27.81593	11.97789	24.57621
S	24.6422	11.95344	19.09892
S	24.6422	11.95344	30.04684
S	30.99372	11.95344	19.09892
S	30.99372	11.95344	30.04684
S	24.64138	11.97822	13.62753
S	24.64138	11.97822	24.57545
S	30.9929	11.97822	13.62753
S	30.9929	11.97822	24.57545
Mo	23.05471	10.27134	18.179
Mo	23.05471	10.27134	29.12682
Mo	29.40618	10.27134	18.179
Mo	29.40618	10.27134	29.12682
Mo	23.05297	10.28004	12.68428
Mo	23.05297	10.28004	23.63211
Mo	29.40448	10.28004	12.68428
Mo	29.40448	10.28004	23.63211
Mo	26.22994	10.27242	18.17918
Mo	26.22994	10.27242	29.127
Mo	32.58141	10.27242	18.17918
Mo	32.58141	10.27242	29.127
Mo	26.22863	10.27917	12.68848
Mo	26.22863	10.27917	23.6364
Mo	32.58015	10.27917	12.68848
Mo	32.58015	10.27917	23.6364
S	23.05771	8.58555	16.35132
S	23.05771	8.58555	27.29923
S	29.40923	8.58555	16.35132
S	29.40923	8.58555	27.29923
S	23.052	8.5323	10.89432
S	23.052	8.5323	21.84224
S	23.052	8.5323	32.79015

S	29.40347	8.5323	10.89432
S	29.40347	8.5323	21.84224
S	29.40347	8.5323	32.79015
S	26.23003	8.58657	16.35136
S	26.23003	8.58657	27.29928
S	32.58155	8.58657	16.35136
S	32.58155	8.58657	27.29928
S	26.22341	8.54193	10.89285
S	26.22341	8.54193	21.84081
S	26.22341	8.54193	32.78863
S	32.57497	8.54193	10.89285
S	32.57497	8.54193	21.84081
S	32.57497	8.54193	32.78863
S	23.058	11.98674	16.36924
S	23.058	11.98674	27.31706
S	29.40951	11.98674	16.36924
S	29.40951	11.98674	27.31706
S	23.05273	11.99865	10.87345
S	23.05273	11.99865	21.82127
S	23.05273	11.99865	32.76919
S	29.40429	11.99865	10.87345
S	29.40429	11.99865	21.82127
S	29.40429	11.99865	32.76919
S	26.22994	11.98704	16.36852
S	26.22994	11.98704	27.31635
S	32.58141	11.98704	16.36852
S	32.58141	11.98704	27.31635
S	26.22592	11.98689	10.87175
S	26.22592	11.98689	21.81966
S	26.22592	11.98689	32.76762
S	32.57749	11.98689	10.87175
S	32.57749	11.98689	21.81966
Au	32.87748	8.25	7.136912
Au	32.87748	12.32826	7.136912
Au	24.72098	8.25	7.136912
Au	24.72098	12.32826	7.136912
Au	28.79918	8.25	7.136912
Au	28.79918	12.32826	7.136912
Au	22.68188	10.28913	7.136912
Au	26.76008	10.28913	7.136912
Au	30.83838	10.28913	7.136912
Au	22.68188	8.25	5.097774
Au	22.68188	8.25	9.176005
Au	22.68188	12.32826	5.097774

Au	22.68188	12.32826	9.176005
Au	26.76008	8.25	5.097774
Au	26.76008	8.25	9.176005
Au	26.76008	12.32826	5.097774
Au	26.76008	12.32826	9.176005
Au	30.83838	8.25	5.097774
Au	30.83838	8.25	9.176005
Au	30.83838	12.32826	5.097774
Au	30.83838	12.32826	9.176005
Au	32.87748	10.28913	5.097774
Au	32.87748	10.28913	9.176005
Au	24.72098	10.28913	5.097774
Au	24.72098	10.28913	9.176005
Au	28.79918	10.28913	5.097774
Au	28.79918	10.28913	9.176005
Au	33.03625	8.26407	36.71825
Au	33.03625	12.3423	36.71825
Au	24.87976	8.26407	36.71825
Au	24.87976	12.3423	36.71825
Au	28.958	8.26407	36.71825
Au	28.958	12.3423	36.71825
Au	22.84066	10.30317	36.71825
Au	26.91886	10.30317	36.71825
Au	30.99715	10.30317	36.71825
Au	22.84066	8.26407	38.75739
Au	22.84066	8.26407	34.7791
Au	22.84066	12.3423	38.75739
Au	22.84066	12.3423	34.67916
Au	26.91886	8.26407	38.75739
Au	26.91886	8.26407	34.67916
Au	26.91886	12.3423	38.75739
Au	26.91886	12.3423	34.67916
Au	30.99715	8.26407	38.75739
Au	30.99715	8.26407	34.67916
Au	30.99715	12.3423	38.75739
Au	30.99715	12.3423	34.67916
Au	33.03625	10.30317	38.75739
Au	33.03625	10.30317	34.67916
Au	24.87976	10.30317	38.75739
Au	24.87976	10.30317	34.67916
Au	28.958	10.30317	38.75739
Au	28.958	10.30317	34.67916
S	32.57749	11.98689	32.76762
H	21.83211	11.3004	21.08965



H	21.83211	11.3004	15.58188
H	21.83211	11.3004	26.59738
H	21.85982	9.19803	21.07808
H	21.85982	9.19803	15.57035
H	21.85982	9.19803	26.58585
H	33.60785	11.41179	21.0817
H	33.60785	11.41179	15.57393
H	33.60785	11.41179	26.58942
H	33.62884	9.30279	21.08201
H	33.62884	9.30279	15.57424
H	33.62884	9.30279	26.58973
H	33.40676	9.36492	13.49407
H	33.40676	9.36492	24.50957
H	33.40676	9.36492	19.00184
H	33.40676	9.36492	30.01734
H	22.05767	11.23608	13.49854
H	22.05767	11.23608	24.51404
H	22.05767	11.23608	19.00627
H	22.05767	11.23608	30.02176
H	22.07537	9.26736	13.4955
H	22.07537	9.26736	24.511
H	22.07537	9.26736	19.00327
H	22.07537	9.26736	30.01877
H	33.39292	11.33295	13.49823
H	33.39292	11.33295	24.51372
H	33.39292	11.33295	19.00595
H	33.39292	11.33295	30.02145
Au	32.87748	8.25	3.058662
Au	32.87748	12.32826	3.058662
Au	24.72098	8.25	3.058662
Au	24.72098	12.32826	3.058662
Au	28.79918	8.25	3.058662
Au	28.79918	12.32826	3.058662
Au	22.68188	10.28913	3.058662
Au	26.76008	10.28913	3.058662
Au	30.83838	10.28913	3.058662
Au	22.68188	8.25	1.019538
Au	22.68188	12.32826	1.019538
Au	26.76008	8.25	1.019538
Au	26.76008	12.32826	1.019538
Au	30.83838	8.25	1.019538
Au	30.83838	12.32826	1.019538
Au	32.87748	10.28913	1.019538
Au	24.72098	10.28913	1.019538

Au	28.79918	10.28913	1.019538
Au	33.03625	8.26407	40.79648
Au	33.03625	12.3423	40.79648
Au	24.87976	8.26407	40.79648
Au	24.87976	12.3423	40.79648
Au	28.958	8.26407	40.79648
Au	28.958	12.3423	40.79648
Au	22.84066	10.30317	40.79648
Au	26.91886	10.30317	40.79648
Au	30.99715	10.30317	40.79648
Au	22.84066	8.26407	42.83557
Au	22.84066	12.3423	42.83557
Au	26.91886	8.26407	42.83557
Au	26.91886	12.3423	42.83557
Au	30.99715	8.26407	42.83557
Au	30.99715	12.3423	42.83557
Au	33.03625	10.30317	42.83557
Au	24.87976	10.30317	42.83557
Au	28.958	10.30317	42.83557
Au	3.058662	16.73544	21.84536
Au	3.058662	14.69631	19.80627
Au	3.058662	14.69631	23.8845
Au	3.058662	18.77457	19.80627
Au	3.058662	18.77457	23.8845
Au	1.019538	14.69631	21.84536
Au	1.019538	18.77457	21.84536
Au	1.019538	16.73544	19.80627
Au	1.019538	16.73544	23.8845
Au	52.61544	16.73544	21.84536
Au	52.61544	14.69631	19.80627
Au	52.61544	14.69631	23.8845
Au	52.61544	18.77457	19.80627
Au	52.61544	18.77457	23.8845
Au	54.65464	14.69631	21.84536
Au	54.65464	18.77457	21.84536
Au	54.65464	16.73544	19.80627
Au	54.65464	16.73544	23.8845

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Table S2 Cartesian coordinates of the graphene/ $V_7(\text{Bz})_8$  vdW junction

Atom	X	Y	Z
Au	49.57631	7.631314	25.58059
Au	49.57631	11.70957	25.58059
Au	49.57631	9.670443	23.54152
Au	49.57631	9.670443	27.61975
Au	47.53712	9.670443	25.58059
Au	47.53712	7.631314	23.54152
Au	47.53712	7.631314	27.61975
Au	47.53712	11.70957	23.54152
Au	47.53712	11.70957	27.61975
Au	5.097728	7.631314	25.58059
Au	5.097728	11.70957	25.58059
Au	5.097728	9.670443	23.54152
Au	5.097728	9.670443	27.61975
Au	7.136851	9.670443	25.58059
Au	7.136851	7.631314	23.54152
Au	7.136851	7.631314	27.61975
Au	7.136851	11.70957	23.54152
Au	7.136851	11.70957	27.61975
C	21.84931	5.099985	46.18173
C	24.3105	5.099985	46.18173
C	26.77175	5.099985	46.18173
C	29.23294	5.099985	46.18173
C	31.69413	5.099985	46.18173
H	33.86873	5.099985	46.01624
H	20.90534	5.099985	45.63669
C	23.07988	5.099985	45.4712
C	25.54113	5.099985	45.4712
C	28.00231	5.099985	45.4712
C	30.4635	5.099985	45.4712
C	32.92475	5.099985	45.4712
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C	29.23294	5.099985	43.33975
C	31.69413	5.099985	43.33975

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C	29.23294	5.099985	4.973394
C	31.69413	5.099985	4.973394
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H	20.90534	5.099985	5.518381
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H	16.72561	12.3924	25.55944
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H	16.71751	11.03329	23.22219
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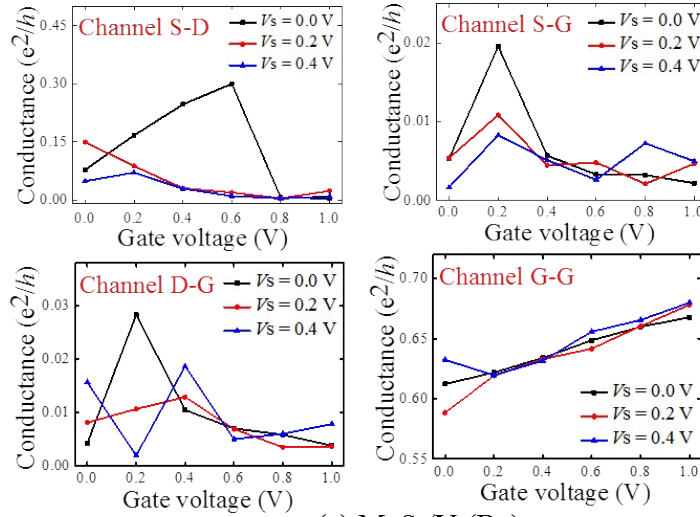
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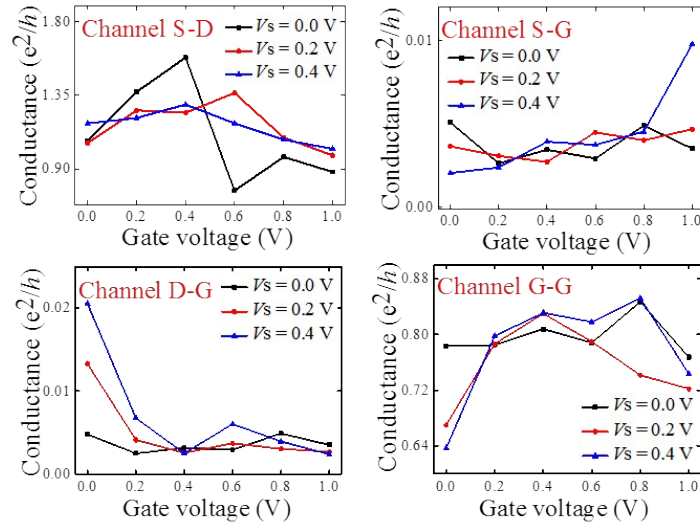
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C	21.84931	5.099985	50.4446
C	24.3105	5.099985	50.4446
C	26.77175	5.099985	50.4446
C	29.23294	5.099985	50.4446
C	31.69413	5.099985	50.4446
Au	3.058666	9.670443	25.58059
Au	3.058666	7.631314	23.54152
Au	3.058666	7.631314	27.61975
Au	3.058666	11.70957	23.54152
Au	3.058666	11.70957	27.61975
Au	1.019534	7.631314	25.58059
Au	1.019534	11.70957	25.58059
Au	1.019534	9.670443	23.54152
Au	1.019534	9.670443	27.61975
Au	51.61543	9.670443	25.58059
Au	51.61543	7.631314	23.54152
Au	51.61543	7.631314	27.61975
Au	51.61543	11.70957	23.54152
Au	51.61543	11.70957	27.61975
Au	53.65462	7.631314	25.58059
Au	53.65462	11.70957	25.58059
Au	53.65462	9.670443	23.54152

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(a)  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$



(b)  $\text{graphene}/\text{V}_7(\text{Bz})_8$

Figure S1. Conductance for Channel S-D, Channel S-G, Channel D-G, and Channel G-G as a function of  $V_G$  at fixed values of  $V_S=0.0, 0.2$ , or  $0.4$  V of the four-terminal  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$  and  $\text{graphene}/\text{V}_7(\text{Bz})_8$  devices. (a) and (b) are for the  $\text{MoS}_2/\text{V}_7(\text{Bz})_8$  and  $\text{graphene}/\text{V}_7(\text{Bz})_8$  devices, respectively. This figure corresponds to Figure 3, and here, the vertical-axis scales are adapted to their content.