Supporting information: Determination of scattering time and of valley occupation in transition-metal dichalcogenides doped by field effect

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(Dated: January 27, 2016)

I. COMPUTATIONAL DETAILS

All electronic-structure calculations have been performed within the framework of DFT as implemented in the Quantum ESPRESSO package[1] which uses a plane-wave basis set to describe the valence-electron wave function and charge density. We employed full-relativistic, projector augmented wave potentials[2]. We chose the Perdew-Burke-Ernzerhof functional[3] for the exchange-correlation energy and furthermore included dispersion corrections[4]. For the molybdenum containing dichalcogenides we used a cutoff of 50 Ry and 410 Ry (1 Ry $\approx$ 13.6 eV) for the wave functions and the charge density, respectively, while for the tungsten dichalcogenides we chose 55 Ry/410 Ry. The Brillouin zone integration has been performed with a Monkhorst-Pack grid[5] of $64 \times 64 \times 1$ **k** points together with a Gaussian broadening of 0.002 Ry $\approx$ 27 meV. Afterwards, we performed an additional non-self-consistent calculation on a denser **k**-point grid of at least $90 \times 90 \times 1$ points starting from the converged charge density. The self-consistent solution of the Kohn-Sham equations was obtained when the total energy changed by less than 10^{-9} Ry and the maximum force on all atoms was less than 5×10^{-4} Ry a_0^{-1} ($a_0 \approx 0.529177$ Å is the Bohr radius). For the trilayer systems of MoS_2 and WS_2 we reduced the force cutoff to 1×10^{-4} Ry a_0^{-1}. We used the same unit-cell sizes as in Ref. 6.

For the FET setup we used our method described in Ref. 7. The dipole for the dipole correction[7,8] was placed at $z_{\rm dip} = d_{\rm dip}/2$ with $d_{\rm dip} = 0.01\,L$ and L being the unit-cell size in the direction perpendicular to the 2D plane – L changed for the different calculations and was between 34 Å and 48 Å. The charged plane modeling the gate electrode[7] was placed close to the dipole at $z_{\rm mono} = 0.011\,L$. A potential barrier with a height of $V_0 = 2$ Ry and a width of $d_b = 0.1\,L$ was used in order to prevent the ions from moving too close to the gate electrode. The final results were found to be independent of the separation of the dipole planes, as well as the barrier height and width as long as it is high or thick enough to ensure that the electron density at the position of the dipole and the gate electrode is zero, $\rho^e\left(z_{\rm mono}\right) = \rho^e\left(z_{\rm dip}\right) = 0$. In order to calculate the conductivity tensors $\sigma_{\alpha\beta}(T;E_F)$ and $\sigma_{\alpha\beta\gamma}(T;E_F)$, we used the BoltzTraP code[9]. We fitted the band structure for each doping of the different TMDs by using 55-times more plane waves than bands. We checked the convergence by calculating $\sigma_{\alpha\beta}(T;E_F)$ with increasing number of **k** points and found that the results do not change when increasing the **k**-point grid from $64 \times 64 \times 1$ to the denser grid of the non-self-consistent calculation.

II. RATIO OF THE MOBILITY TO THE SCATTERING TIME

With the data summarized in the tables and presented in the figures, the transport scattering time can be extracted from the experimental data as presented in Figure 1 of the main text. All calculations were done for $T = 300\,\mathrm{K}$ and using the unit cell as relaxed with PBE+D2[6].

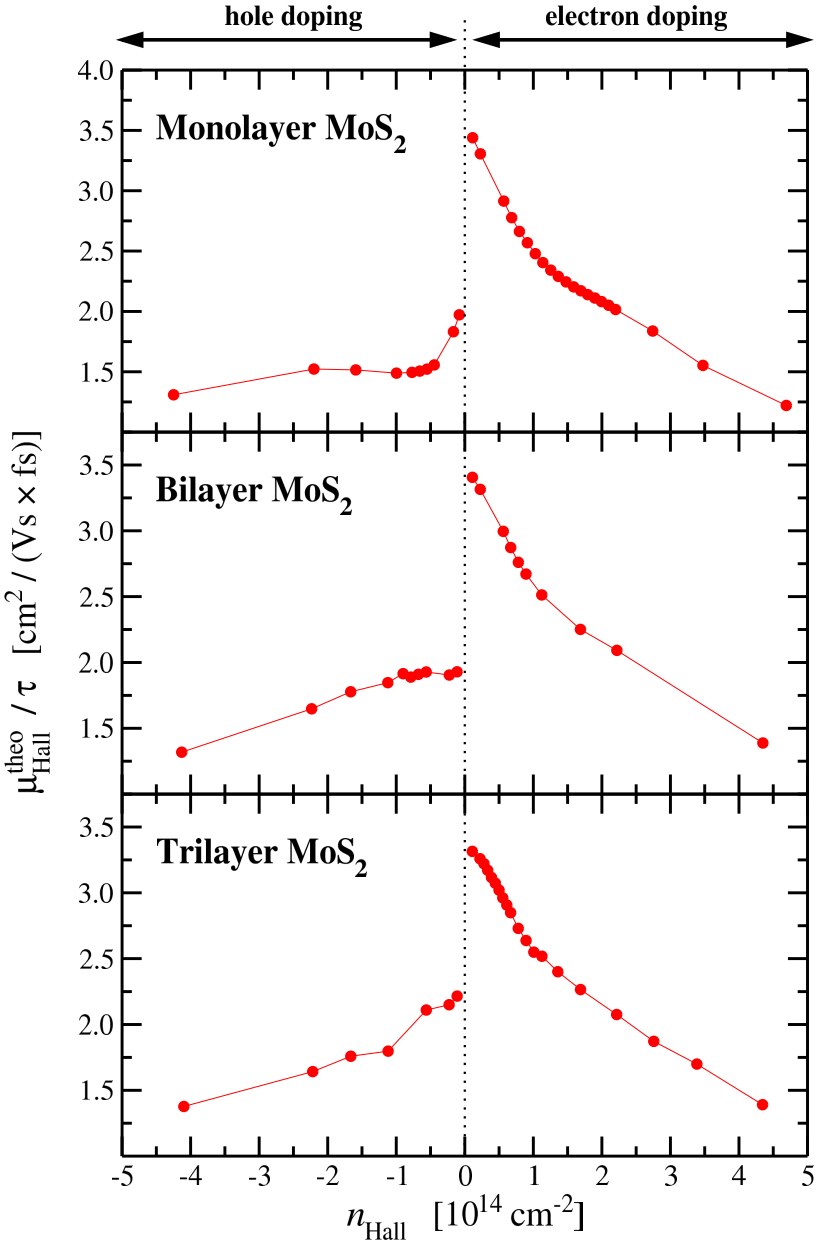

FIG. 1. Ratio of the mobility to the scattering time, $\mu^{\mathrm{theo}}_{\mathrm{Hall}}/\tau$, for doping of MoS_2.

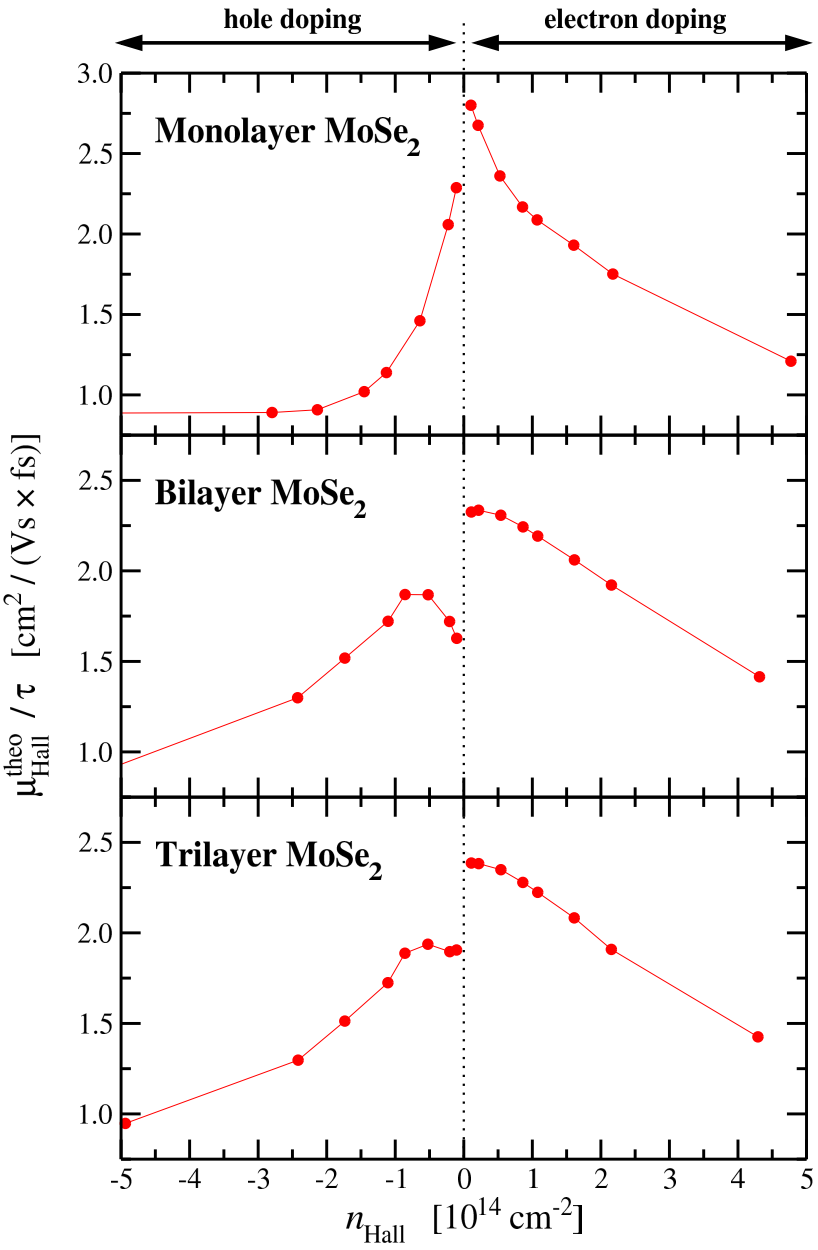

FIG. 2. Ratio of the mobility to the scattering time, $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$, for doping of $MoSe_2$.

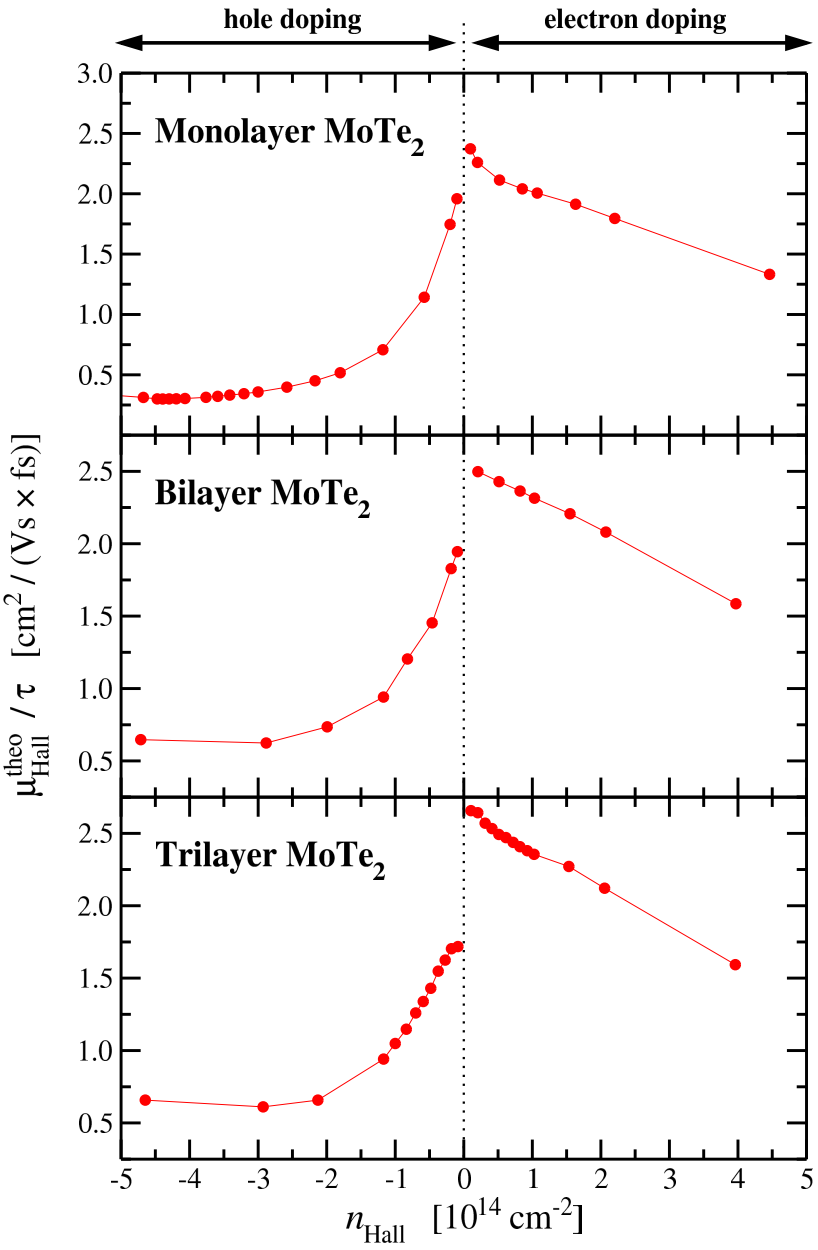

FIG. 3. Ratio of the mobility to the scattering time, $\mu^{\rm theo}_{\rm Hall}/\tau$, for doping of $MoTe_2$.

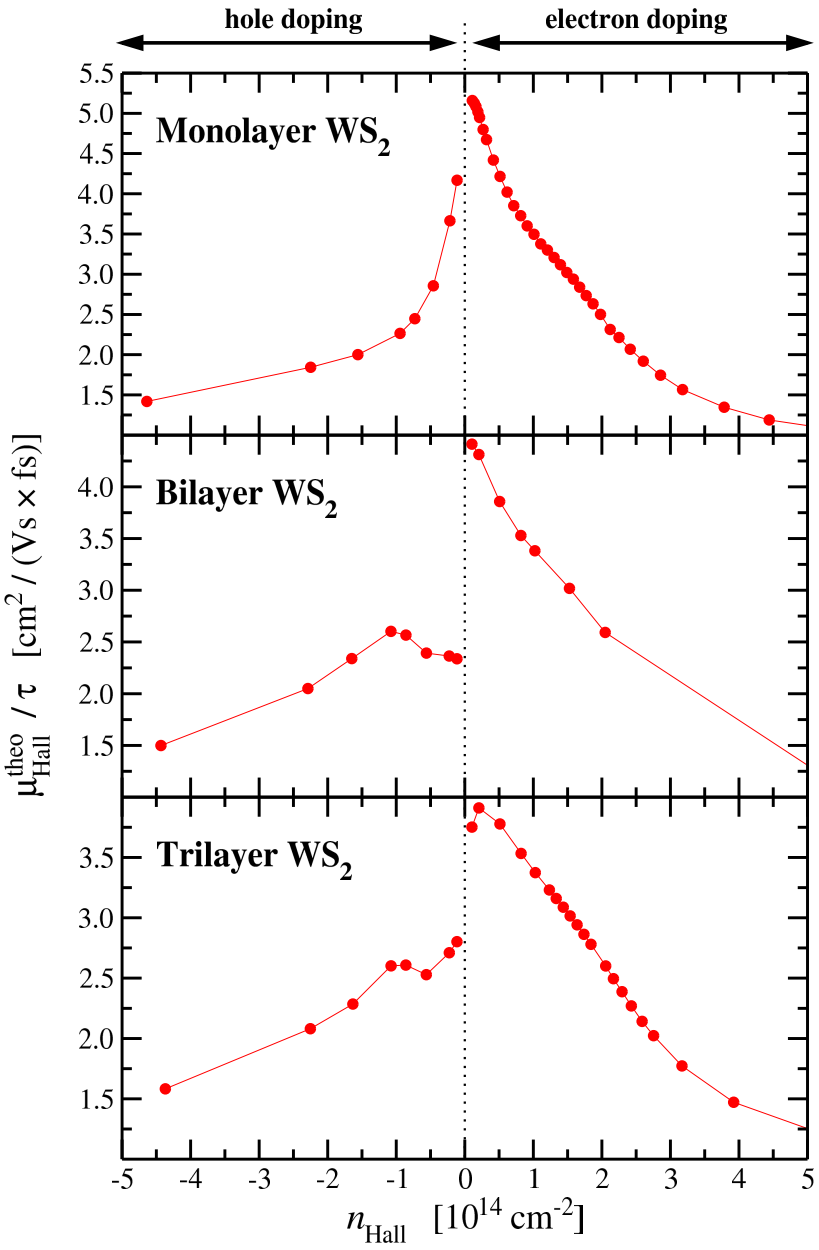

FIG. 4. Ratio of the mobility to the scattering time, $\mu^{\mathrm{theo}}_{\mathrm{Hall}}/\tau$, for doping of WS_2.

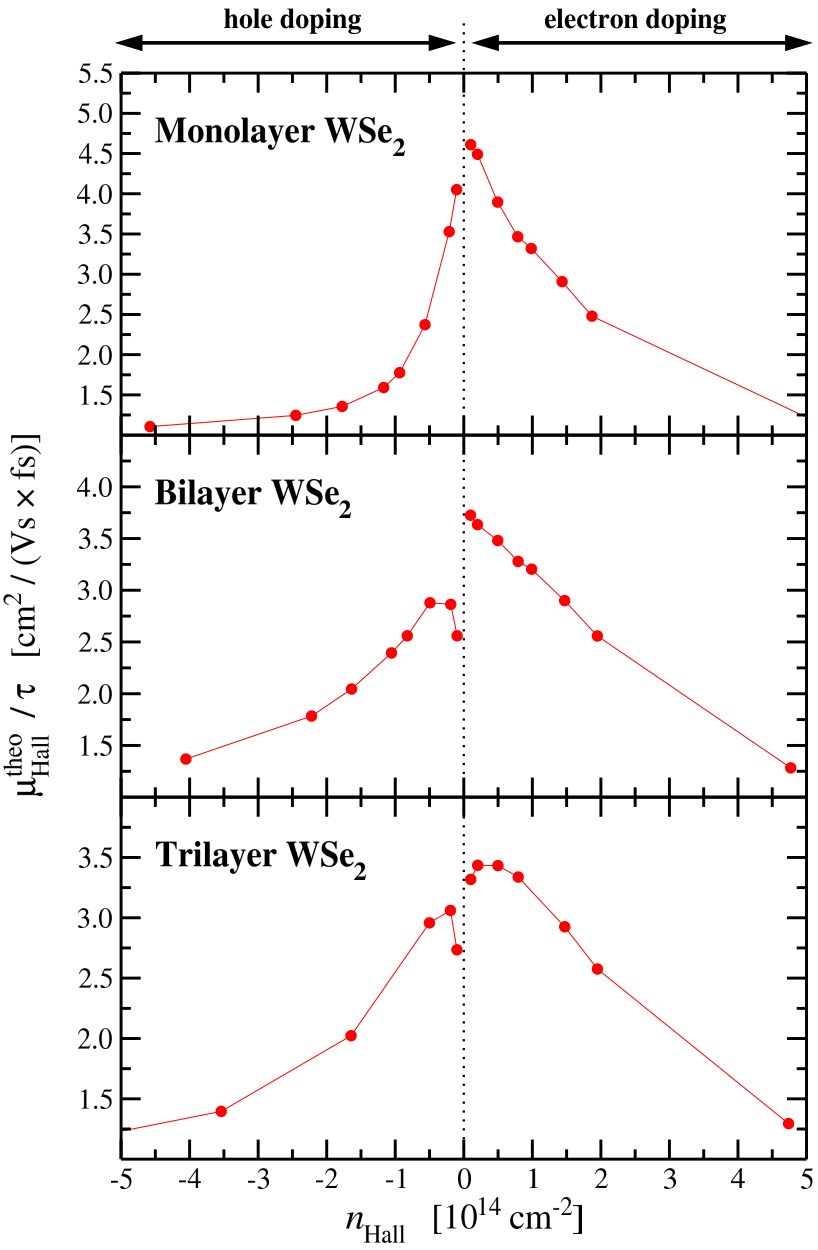

FIG. 5. Ratio of the mobility to the scattering time, $\mu^{\rm theo}_{\rm Hall}/\tau$, for doping of WSe_2.

TABLE I. Ratio of the mobility to the scattering time, $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$, for doping of MoS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ is given in $\mathrm{cm}^2/(\mathrm{V\,s}\times\mathrm{fs})$.

Monolayer		Bilayer		Trilayer	
n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$
-4.2491626	1.3091163	-4.1296552	1.3181378	-4.098818	1.3772912
-2.2011886	1.5225442	-2.2339244	1.6477311	-2.2187374	1.6421734
-1.5893042	1.5155152	-1.6642117	1.7772683	-1.6633634	1.7584128
-0.99733892	1.4881301	-1.1231998	1.8462131	-1.118947	1.7971142
-0.76974118	1.494788	-0.89985239	1.914799	-0.5618741	2.1095822
-0.65771863	1.5051919	-0.7888849	1.888821	-0.22901122	2.1501767
-0.55163215	1.5214138	-0.6777032	1.9100087	-0.1110224	2.215091
-0.4460156	1.5567485	-0.56312938	1.9278586		
-0.16556166	1.8314334	-0.22625942	1.9041743	0.10995963	3.3149139
-0.080191802	1.972332	-0.11270142	1.9288163	0.22156061	3.2586982
				0.27967357	3.2212498
0.11447109	3.439233	0.11152738	3.4064375	0.33361732	3.1715472
0.22717979	3.3062514	0.22604931	3.3146364	0.39049075	3.1162799
0.56806524	2.9143156	0.56093065	2.9960114	0.44608101	3.0728598
0.68428702	2.777262	0.6705943	2.8726889	0.49989295	3.0199042
0.79699679	2.6626637	0.7809586	2.7604433	0.55459743	2.9615938
0.91326164	2.5693534	0.89273174	2.6712793	0.612537	2.9069953
1.0285618	2.4780937	1.1223905	2.5130625	0.66906237	2.8494044
1.1387553	2.4048675	1.6864759	2.2511215	0.7805717	2.7298295
1.2548959	2.341795	2.2188961	2.0915386	0.89396019	2.637666
1.3646634	2.2903715	4.3488299	1.3879042	1.0072688	2.549273
1.4778319	2.2447601			1.1263014	2.5180558
1.588172	2.2035174			1.3575356	2.4003868
1.6921762	2.1710605			1.6882634	2.2652913
1.7924943	2.1389658			2.2153162	2.0759193
1.8970672	2.110556			2.7577624	1.8716837
1.9946949	2.0817882			3.385373	1.6991116
2.0979988	2.0506219			4.3441106	1.3902748
2.200607	2.0160187				
2.7410158	1.8370352				
3.4741789	1.5525132				
4.6899383	1.2209722				

TABLE II. $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ for doping of $MoSe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ is given in $\mathrm{cm}^2/(\mathrm{V\,s}\times\mathrm{fs})$.

Monolayer		Bilayer		Trilayer	
n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$
4.7731017	1.2095376	4.3135928	1.4147416	4.2919296	1.4255861
2.1740007	1.7512346	2.1536538	1.9218338	2.1532276	1.9087642
1.6047773	1.9305599	1.614592	2.0607023	1.6118883	2.0829011
1.06965	2.0875163	1.0784851	2.1921824	1.0787673	2.2239184
0.85700705	2.1678165	0.86478195	2.2431461	0.86075675	2.2786271
0.52784856	2.3606444	0.53990246	2.3072667	0.54118178	2.3488712
0.20882683	2.6754158	0.21625638	2.3351134	0.21718596	2.382695
0.10482951	2.8001297	0.10943795	2.3250322	0.10985212	2.3856646
-0.10919585	2.2876721	-0.10345193	1.6274622	-0.10622988	1.9054335
-0.2266871	2.0585169	-0.2068659	1.7202007	-0.20377378	1.8964843
-0.64057209	1.4604964	-0.52061929	1.8683148	-0.52379019	1.9372724
-1.1283666	1.1389651	-0.85704697	1.8691041	-0.85834509	1.8874274
-1.4527003	1.0199095	-1.1047955	1.7213502	-1.1069769	1.7246169
-2.1359692	0.90778421	-1.7359182	1.5178883	-1.7362424	1.512987
-2.7973089	0.89023529	-2.4247998	1.2990235	-2.4176947	1.2971107
-5.192778	0.88730686	-5.0129648	0.92955869	-4.9377152	0.94769545

TABLE III. $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ for doping of $MoTe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ is given in $\mathrm{cm}^2/(\mathrm{V\,s}\times\mathrm{fs})$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$
4.4620591	1.3324162	3.9705544	1.585565	3.9618465	1.5928783
2.2025426	1.795528	2.0731326	2.0803529	2.0542661	2.121062
1.6313633	1.9132088	1.549368	2.2065999	1.5328462	2.2715083
1.0716865	2.005846	1.0309044	2.3144434	1.0251345	2.3549568
0.85378092	2.041081	0.82200827	2.3636689	0.92619229	2.3797412
0.52184321	2.1134603	0.51422428	2.4289004	0.8181898	2.4075392
0.20057799	2.2602097	0.20624584	2.4973874	0.72017951	2.4378342
0.097547599	2.372779			0.61406719	2.4707813
		-0.09308686	1.9451132	0.51177305	2.4919941
-0.099293354	1.9589262	-0.1835839	1.8281098	0.41117527	2.5332023
-0.19965373	1.7463361	-0.46162918	1.4534115	0.31200062	2.5701318
-0.57692017	1.1423125	-0.82214208	1.2042162	0.20405912	2.6422788
-1.1801887	0.70739437	-1.1718632	0.94090915	0.10362789	2.656415
-1.8026589	0.51692203	-1.9935264	0.73559809		
-2.1701622	0.45011927	-2.8829782	0.62361885	-0.085827864	1.7182319
-2.5816873	0.39756332	-4.7128308	0.64690208	-0.17998372	1.7032156
-3.0018669	0.358077			-0.27090748	1.6248757
-3.2069041	0.34310035			-0.37262262	1.5483233
-3.4136277	0.3314773			-0.48212991	1.4296804
-3.5902112	0.32101812			-0.59139557	1.3388434
-3.7614088	0.313493			-0.7013484	1.2598248
-4.0672504	0.30308619			-0.83829488	1.1471534
-4.1935898	0.30080622			-0.99985758	1.0487574
-4.298634	0.2999286			-1.1696198	0.94102643
-4.3931009	0.29959697			-2.1292659	0.65746855
-4.4735689	0.30043331			-2.9264294	0.61125488
-4.6748095	0.31255696			-4.6471898	0.65806975
-6.9799483	0.40588028				

TABLE IV. $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ for doping of WS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ is given in $\mathrm{cm}^2/(\mathrm{V\,s}\times\mathrm{fs})$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$
5.9451187	1.0001519	5.2540225	1.1974425	5.2034001	1.2123278
4.4418238	1.1879715	2.0490091	2.5920018	3.9235511	1.4718003
3.7841895	1.347127	1.5269852	3.0185814	3.1687812	1.7723462
3.1775658	1.5652455	1.0226057	3.3822742	2.7548765	2.0234544
2.8561	1.7449875	0.81866269	3.5291151	2.5875534	2.1420721
2.6044336	1.9186328	0.50848075	3.8576826	2.4296378	2.2701465
2.4141684	2.0677054	0.20564131	4.3120659	2.2947373	2.3873952
2.2500813	2.2131801	0.10373654	4.4129047	2.1691808	2.4956751
2.1217414	2.3127601			2.0553287	2.6009189
1.9800159	2.5003633	-0.11360442	2.3373775	1.8418346	2.780131
1.8708091	2.6323568	-0.22732088	2.3638436	1.7391726	2.8628788
1.7718938	2.7340647	-0.56065269	2.3920776	1.6389206	2.9416379
1.6762202	2.8390185	-0.85870253	2.5662758	1.5368319	3.0157106
1.5846173	2.9392175	-1.0767483	2.6029349	1.4373844	3.0878722
1.4892628	3.0212652	-1.6487975	2.3391736	1.3346483	3.1600452
1.395736	3.1177388	-2.2884839	2.0501036	1.233926	3.2308477
1.3021736	3.2077902	-4.4329284	1.4988338	1.0285453	3.3746177
1.2059799	3.2998479			0.82193897	3.5333373
1.1082159	3.3766862			0.5134167	3.7779927
1.0096871	3.4960482			0.20575059	3.9108741
0.90940289	3.6013727			0.10408891	3.7514795
0.81522236	3.7281411				
0.71454245	3.8512842			-0.11385782	2.8021559
0.61765518	4.0207067			-0.22574283	2.7102099
0.5136024	4.2156342			-0.56095037	2.5290743
0.4172856	4.4194398			-0.8601742	2.6085927
0.31699533	4.6729004			-1.0760957	2.6020078
0.26755249	4.7989229			-1.6331629	2.2855875
0.21545743	4.9482107			-2.2530974	2.0805946
0.19181099	5.0179545			-4.3691497	1.5828835
0.16303181	5.0852625				
0.1381423	5.1256607				
0.11042201	5.1584334				
-0.11293672	4.1677082				
-0.21645275	3.6646053				
-0.45803433	2.8557865				
-0.72866793	2.4475153				
-0.94492107	2.2649458				
-1.5601135	2.0006848				
-2.2487039	1.8432438				
-4.6386124	1.4184785				

TABLE V. $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ for doping of WSe_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ is given in $\mathrm{cm}^2/(\mathrm{V\,s}\times\mathrm{fs})$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$	n_{Hall}	$\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$
5.3796416	1.0690628	4.7701666	1.2828633	4.7387494	1.2948932
1.8705484	2.4782892	1.9484388	2.5577935	1.9499477	2.5755846
1.4346005	2.9082576	1.4716749	2.9004286	1.4735385	2.9254339
0.98360345	3.319316	0.99029849	3.2042304	0.79438521	3.338046
0.78776111	3.4655699	0.79288934	3.2782019	0.49792702	3.4329827
0.49414791	3.8972492	0.49623851	3.4814892	0.20276075	3.4355425
0.20053258	4.4910058	0.19929835	3.6348016	0.10165173	3.3183781
0.10072038	4.6105468	0.098916827	3.7250852		
				-0.10069895	2.7350503
-0.10447814	4.0517287	-0.097819854	2.5600942	-0.19406515	3.0613006
-0.21338905	3.5287098	-0.19052331	2.8642205	-0.50087544	2.9579233
-0.56555008	2.3731784	-0.49230567	2.8787049	-1.6441675	2.0232357
-0.93591402	1.7765088	-0.82473921	2.5598287	-3.5378885	1.3962603
-1.1686202	1.5909742	-1.0538261	2.394079	-5.8117567	1.1395649
-1.774195	1.356287	-1.6377766	2.0447787		
-2.4512037	1.2459518	-2.2216063	1.7839459		
-4.5769638	1.1056685	-4.0546696	1.3684303		

III. DENSITY OF STATES AT THE FERMI ENERGY

Using the ratio $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau$ presented in the last section and DOS_{E_F} summarized in this section, one can fit $\mu_{\mathrm{Hall}}^{\mathrm{theo}}/\tau\ (C \times \mathrm{DOS}_{E_F})^{-1}$ to the experimental mobility $\mu_{\mathrm{Hall}}^{\mathrm{exp}}$. The transport scattering time within the constant-relaxation-time approximation is then given by $\tau = (C \times \mathrm{DOS}_{E_F})^{-1}$ as shown in Figure 2 of the main text. All calculations were done for $T = 300\,\mathrm{K}$ and using the unit cell as relaxed with PBE+D2[6].

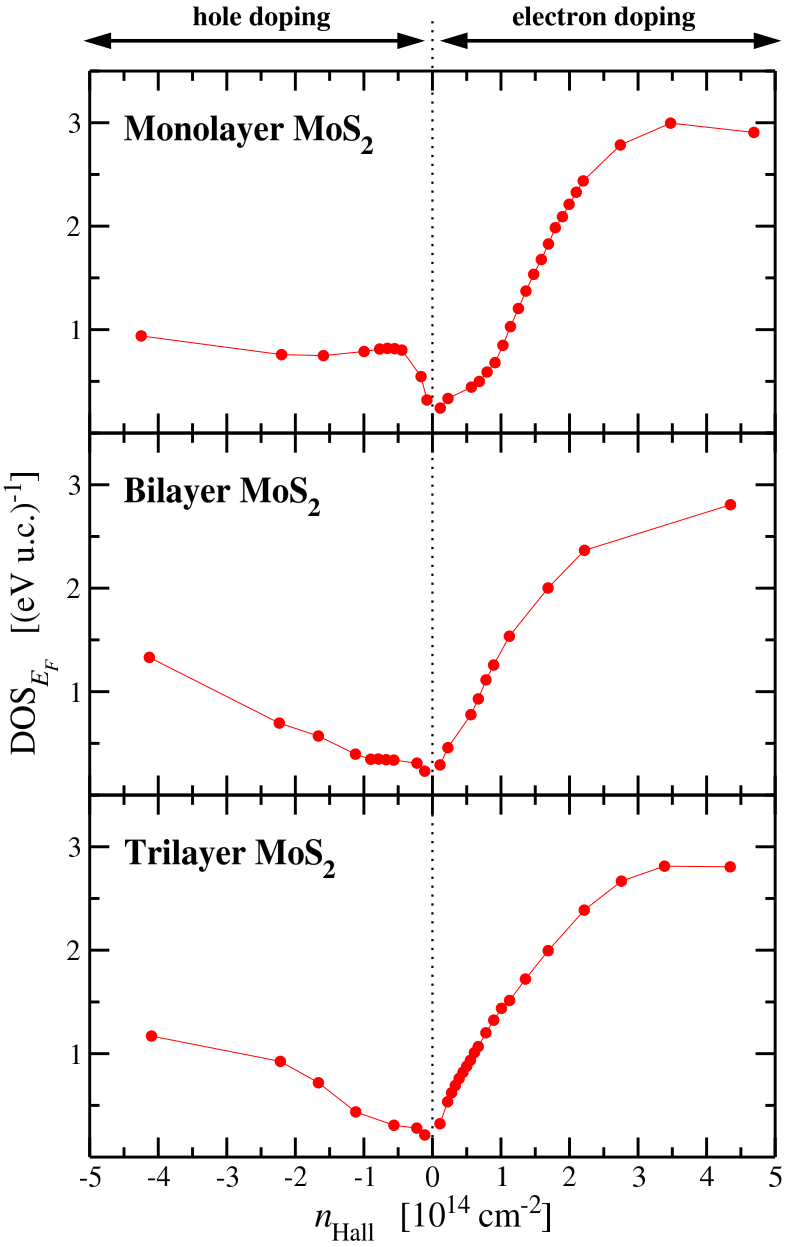

FIG. 6. Density of states at the Fermi energy, DOS_{E_F}, for doping of MoS_2.

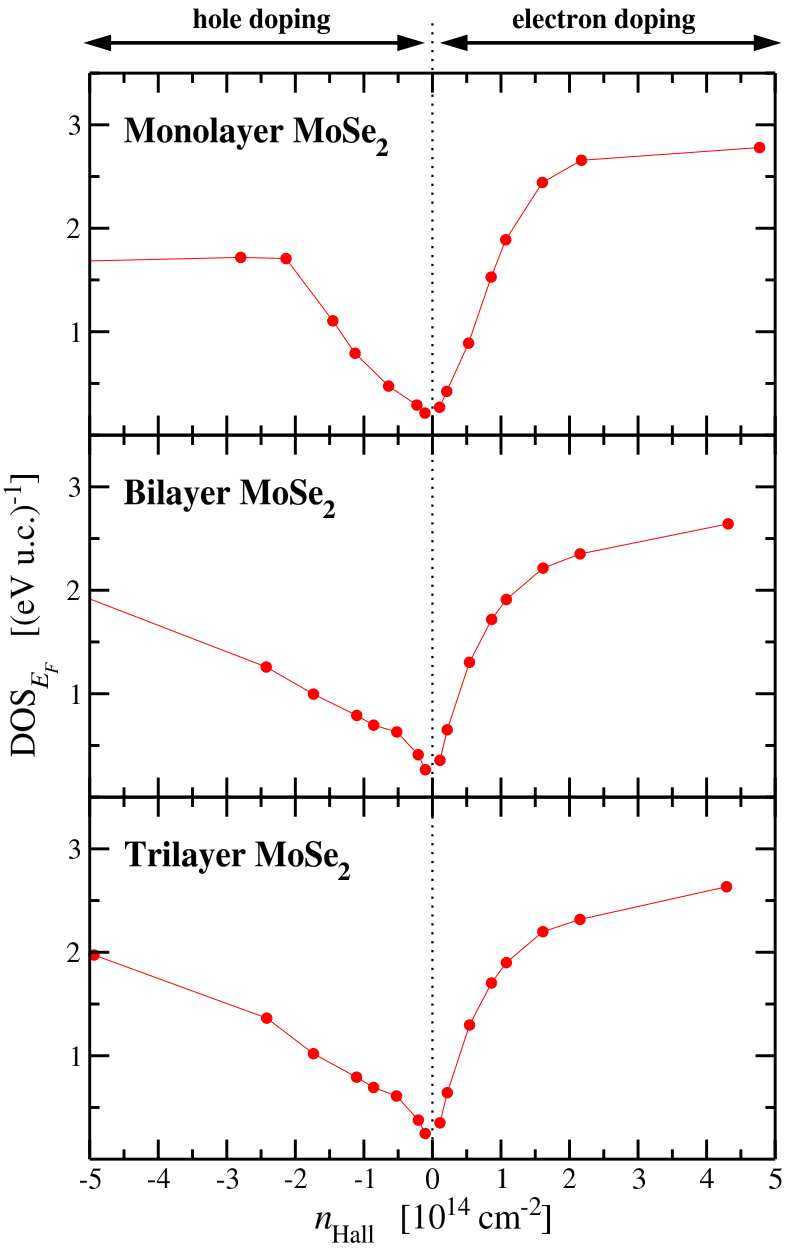

FIG. 7. Density of states at the Fermi energy, DOS_{E_F}, for doping of $MoSe_2$.

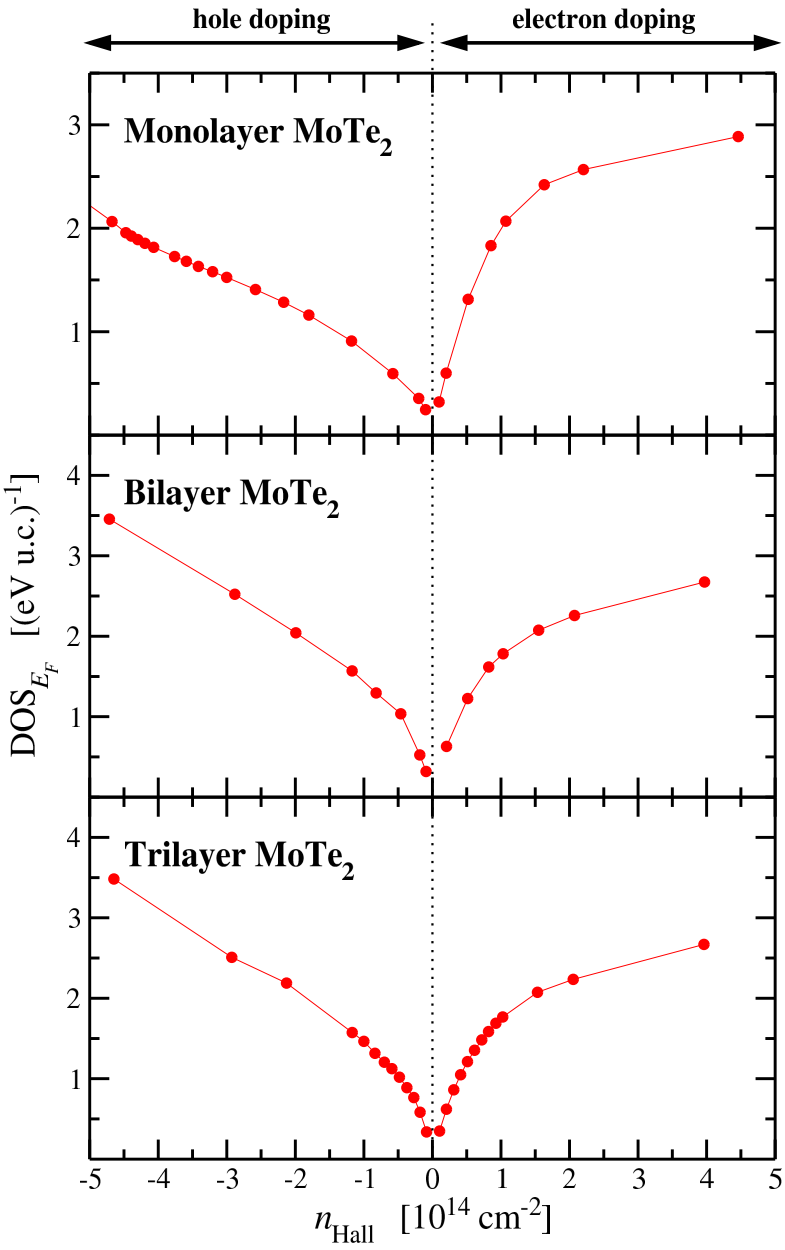

FIG. 8. Density of states at the Fermi energy, DOS_{E_F}, for doping of $MoTe_2$.

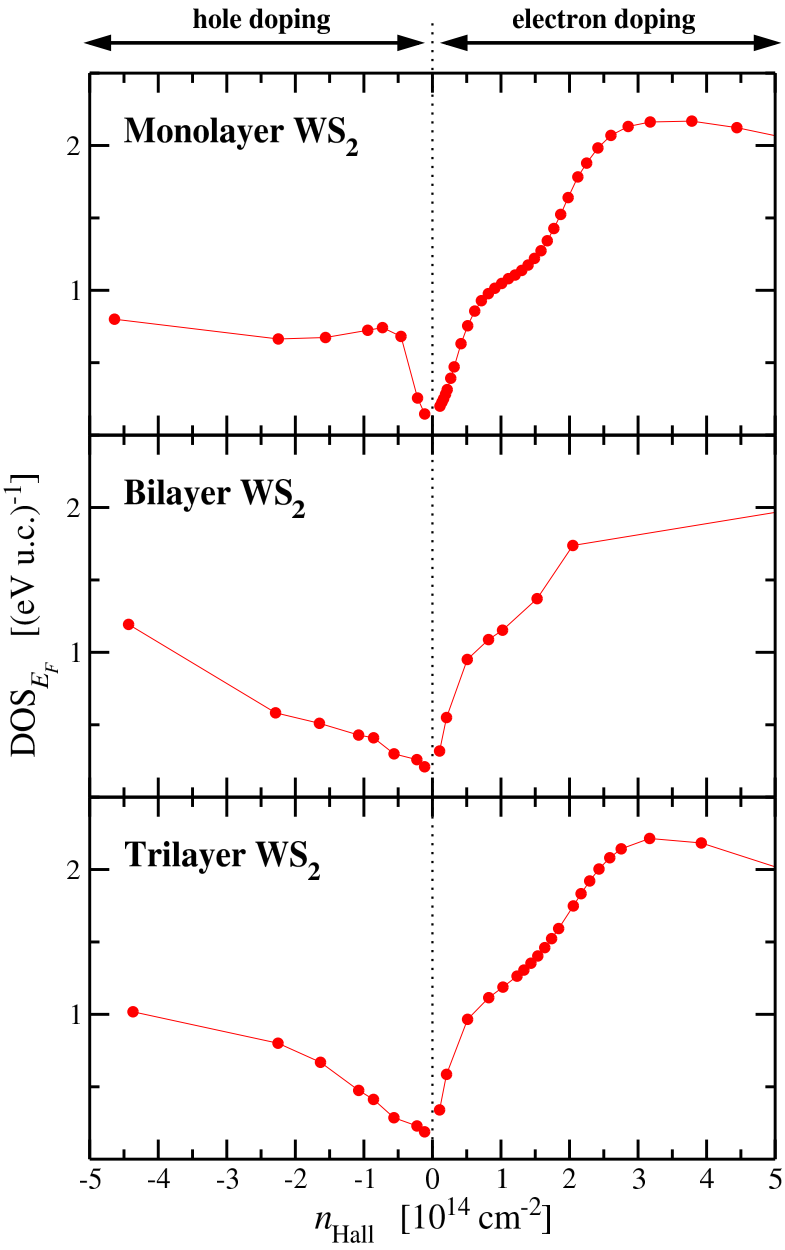

FIG. 9. Density of states at the Fermi energy, DOS_{E_F}, for doping of WS_2.

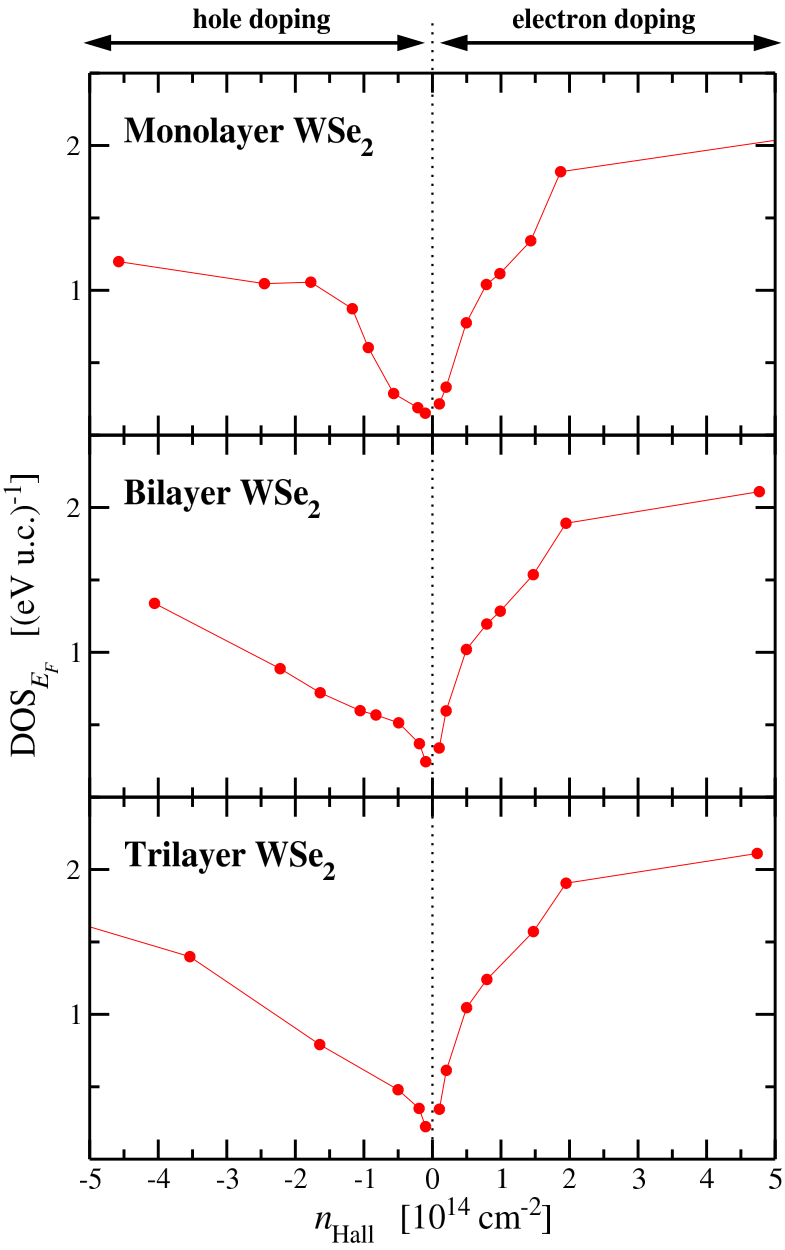

FIG. 10. Density of states at the Fermi energy, DOS_{E_F}, for doping of WSe_2.

TABLE VI. Density of states at the Fermi energy, DOS_{E_F}, for doping of MoS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and DOS_{E_F} is given in $(\mathrm{eV\,u.c.})^{-1}$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}
-4.2491626	0.93942926	-4.2491626	0.93942926	-4.098818	1.1705498
-2.2011886	0.75799833	-2.2011886	0.75799833	-2.2187374	0.92515413
-1.5893042	0.74883783	-1.5893042	0.74883783	-1.6633634	0.71823222
-0.99733892	0.78858321	-0.99733892	0.78858321	-1.118947	0.43667666
-0.76974118	0.8120965	-0.76974118	0.8120965	-0.5618741	0.30789796
-0.65771863	0.81847085	-0.65771863	0.81847085	-0.22901122	0.28061456
-0.55163215	0.81596297	-0.55163215	0.81596297	-0.1110224	0.21377352
-0.4460156	0.80136705	-0.4460156	0.80136705		
-0.16556166	0.54604705	-0.16556166	0.54604705	0.10995963	0.32302197
-0.080191802	0.31975706	-0.080191802	0.31975706	0.22156061	0.5350392
				0.27967357	0.62213274
0.11447109	0.24133266	0.11152738	0.29112686	0.33361732	0.69247366
0.22717979	0.3337826	0.22604931	0.45834663	0.39049075	0.76000029
0.56806524	0.44353419	0.56093065	0.77717262	0.44608101	0.81962456
0.68428702	0.49919567	0.6705943	0.9294258	0.49989295	0.87861251
0.79699679	0.58938961	0.7809586	1.1133433	0.55459743	0.93502816
0.91326164	0.68047913	0.89273174	1.2567259	0.612537	1.0101101
1.0285618	0.84800279	1.1223905	1.5357303	0.66906237	1.0682318
1.1387553	1.0287902	1.6864759	2.001876	0.7805717	1.2016032
1.2548959	1.2045428	2.2188961	2.3654997	0.89396019	1.3232898
1.3646634	1.3727908	4.3488299	2.8069271	1.0072688	1.4384635
1.4778319	1.5340646			1.1263014	1.5141407
1.588172	1.677808			1.3575356	1.7208062
1.6921762	1.8281503			1.6882634	1.9954871
1.7924943	1.9854111			2.2153162	2.3879127
1.8970672	2.0924523			2.7577624	2.6681524
1.9946949	2.2115691			3.385373	2.8128959
2.0979988	2.3276244			4.3441106	2.8064114
2.200607	2.4373525				
2.7410158	2.785399				
3.4741789	2.995717				
4.6899383	2.9061386				

TABLE VII. DOS_{E_F} for doping of $MoSe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and DOS_{E_F} is given in $(\mathrm{eV\,u.c.})^{-1}$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}
4.7731017	2.7807157	4.3135928	2.6418069	4.2919296	2.6332903
2.1740007	2.6574883	2.1536538	2.351284	2.1532276	2.3177747
1.6047773	2.4424274	1.614592	2.2140381	1.6118883	2.1993495
1.06965	1.8884774	1.0784851	1.911334	1.0787673	1.9002341
0.85700705	1.5278947	0.86478195	1.7185304	0.86075675	1.7030959
0.52784856	0.88903723	0.53990246	1.3034096	0.54118178	1.2965041
0.20882683	0.42264904	0.21625638	0.65097291	0.21718596	0.64281295
0.10482951	0.26979462	0.10943795	0.35589382	0.10985212	0.35132009
-0.10919585	0.2124746	-0.10345193	0.26512381	-0.10622988	0.24779577
-0.2266871	0.29017863	-0.2068659	0.40945908	-0.20377378	0.37760267
-0.64057209	0.47387631	-0.52061929	0.63020649	-0.52379019	0.6105696
-1.1283666	0.79154374	-0.85704697	0.69619512	-0.85834509	0.69302579
-1.4527003	1.1051543	-1.1047955	0.78945494	-1.1069769	0.79242727
-2.1359692	1.7066282	-1.7359182	0.99622461	-1.7362424	1.0193987
-2.7973089	1.7185233	-2.4247998	1.2577553	-2.4176947	1.3627911
-5.192778	1.6810151	-5.0129648	1.9196259	-4.9377152	1.9742263

TABLE VIII. DOS_{E_F} for doping of $MoTe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and DOS_{E_F} is given in $(\mathrm{eV\,u.c.})^{-1}$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}
4.4620591	2.8866004	3.9705544	2.6739855	3.9618465	2.6697531
2.2025426	2.5673459	2.0731326	2.2581407	2.0542661	2.2347194
1.6313633	2.420305	1.549368	2.0749148	1.5328462	2.0743894
1.0716865	2.0681986	1.0309044	1.7819364	1.0251345	1.7676272
0.85378092	1.8319485	0.82200827	1.6173518	0.92619229	1.6900406
0.52184321	1.3129504	0.51422428	1.2251369	0.8181898	1.5856623
0.20057799	0.59921436	0.20624584	0.63036132	0.72017951	1.4828257
0.097547599	0.32096512			0.61406719	1.3540907
		-0.09308686	0.31884419	0.51177305	1.2117307
-0.099293354	0.24623594	-0.1835839	0.52397129	0.41117527	1.0489048
-0.19965373	0.35487395	-0.46162918	1.0353469	0.31200062	0.86190579
-0.57692017	0.59418587	-0.82214208	1.2955665	0.20405912	0.6207076
-1.1801887	0.91008338	-1.1718632	1.5693831	0.10362789	0.3495761
-1.8026589	1.160887	-1.9935264	2.0424233		
-2.1701622	1.2848936	-2.8829782	2.5221354	-0.085827864	0.3383641
-2.5816873	1.4071568	-4.7128308	3.4549528	-0.17998372	0.58316093
-3.0018669	1.5253759			-0.27090748	0.76600932
-3.2069041	1.5798611			-0.37262262	0.8886177
-3.4136277	1.6306607			-0.48212991	1.0191428
-3.5902112	1.680704			-0.59139557	1.124683
-3.7614088	1.7271046			-0.7013484	1.2051703
-4.0672504	1.815376			-0.83829488	1.3157665
-4.1935898	1.8543982			-0.99985758	1.4638533
-4.298634	1.8901231			-1.1696198	1.5738786
-4.3931009	1.9242307			-2.1292659	2.1886979
-4.4735689	1.9564825			-2.9264294	2.5087033
-4.6748095	2.064988			-4.6471898	3.4824073
-6.9799483	3.1642051				

TABLE IX. DOS_{E_F} for doping of WS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and DOS_{E_F} is given in $(\mathrm{eV\,u.c.})^{-1}$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}
5.9451187	1.9735492	5.2540225	1.9856015	5.2034001	1.9872
4.4418238	2.1231651	2.0490091	1.7377843	3.9235511	2.1836395
3.7841895	2.1688431	1.5269852	1.3706235	3.1687812	2.2143899
3.1775658	2.1625674	1.0226057	1.1527249	2.7548765	2.1428383
2.8561	2.1316111	0.81866269	1.088044	2.5875534	2.0814017
2.6044336	2.0695157	0.50848075	0.95068088	2.4296378	2.0036632
2.4141684	1.9835268	0.20564131	0.55005211	2.2947373	1.9211306
2.2500813	1.878449	0.10373654	0.3187414	2.1691808	1.8331947
2.1217414	1.7831585			2.0553287	1.7484219
1.9800159	1.6404029	-0.11360442	0.20963741	1.8418346	1.5922391
1.8708091	1.5237992	-0.22732088	0.25916378	1.7391726	1.5227917
1.7718938	1.4270336	-0.56065269	0.29907605	1.6389206	1.4603555
1.6762202	1.3424727	-0.85870253	0.40987766	1.5368319	1.4032554
1.5846173	1.2731014	-1.0767483	0.42855554	1.4373844	1.3531031
1.4892628	1.2206222	-1.6487975	0.51012481	1.3346483	1.3055978
1.395736	1.174212	-2.2884839	0.58225024	1.233926	1.2638171
1.3021736	1.1374688	-4.4329284	1.1931131	1.0285453	1.1881775
1.2059799	1.1054712			0.82193897	1.1147851
1.1082159	1.0806142			0.5134167	0.96538138
1.0096871	1.0475543			0.20575059	0.58529085
0.90940289	1.0142432			0.10408891	0.34041816
0.81522236	0.97737117				
0.71454245	0.92852544			-0.11385782	0.18836662
0.61765518	0.85697256			-0.22574283	0.22946824
0.5136024	0.7550625			-0.56095037	0.28587074
0.4172856	0.63138589			-0.8601742	0.41222491
0.31699533	0.47103672			-1.0760957	0.47496464
0.26755249	0.39302699			-1.6331629	0.66864805
0.21545743	0.31465281			-2.2530974	0.80065533
0.19181099	0.28237584			-4.3691497	1.0176318
0.16303181	0.25075071				
0.1381423	0.2269806				
0.11042201	0.20019183				
-0.11293672	0.14620371				
-0.21645275	0.25595483				
-0.45803433	0.68172941				
-0.72866793	0.74261896				
-0.94492107	0.72385898				
-1.5601135	0.67389038				
-2.2487039	0.66363103				
-4.6386124	0.8003341				

TABLE X. DOS_{E_F} for doping of WSe_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and DOS_{E_F} is given in $(\mathrm{eV\,u.c.})^{-1}$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}	n_{Hall}	DOS_{E_F}
5.3796416	2.0619887	4.7701666	2.1097187	4.7387494	2.111284
1.8705484	1.818715	1.9484388	1.8912744	1.9499477	1.9053643
1.4346005	1.3424264	1.4716749	1.5364521	1.4735385	1.5712444
0.98360345	1.1150549	0.99029849	1.2841241	0.79438521	1.2405282
0.78776111	1.0398299	0.79288934	1.1957024	0.49792702	1.0462165
0.49414791	0.77562143	0.49623851	1.0199261	0.20276075	0.61322831
0.20053258	0.33110253	0.19929835	0.59596766	0.10165173	0.34482837
0.10072038	0.21545353	0.098916827	0.33949997		
				-0.10069895	0.22483572
-0.10447814	0.15162653	-0.097819854	0.24468089	-0.19406515	0.34999675
-0.21338905	0.18951007	-0.19052331	0.36935918	-0.50087544	0.47924454
-0.56555008	0.28715786	-0.49230567	0.51323733	-1.6441675	0.79111737
-0.93591402	0.60435228	-0.82473921	0.56719	-3.5378885	1.3980993
-1.1686202	0.87311691	-1.0538261	0.59705423	-5.8117567	1.7192662
-1.774195	1.0560942	-1.6377766	0.72108132		
-2.4512037	1.0457829	-2.2216063	0.88741802		
-4.5769638	1.1978891	-4.0546696	1.3383787		

IV. AVERAGE SQUARED VELOCITY

Using the transport scattering time extracted from the experimental data, one can calculate within the constant-relaxation-time approximation the mean-free path as $l = \langle v \rangle \tau \approx \sqrt{2\langle v_x^2 \rangle} \times \tau$. Here, we present the average squared velocity which is needed to determine l. All calculations were done for $T = 300\,\mathrm{K}$ and using the unit cell as relaxed with PBE+D2[6].

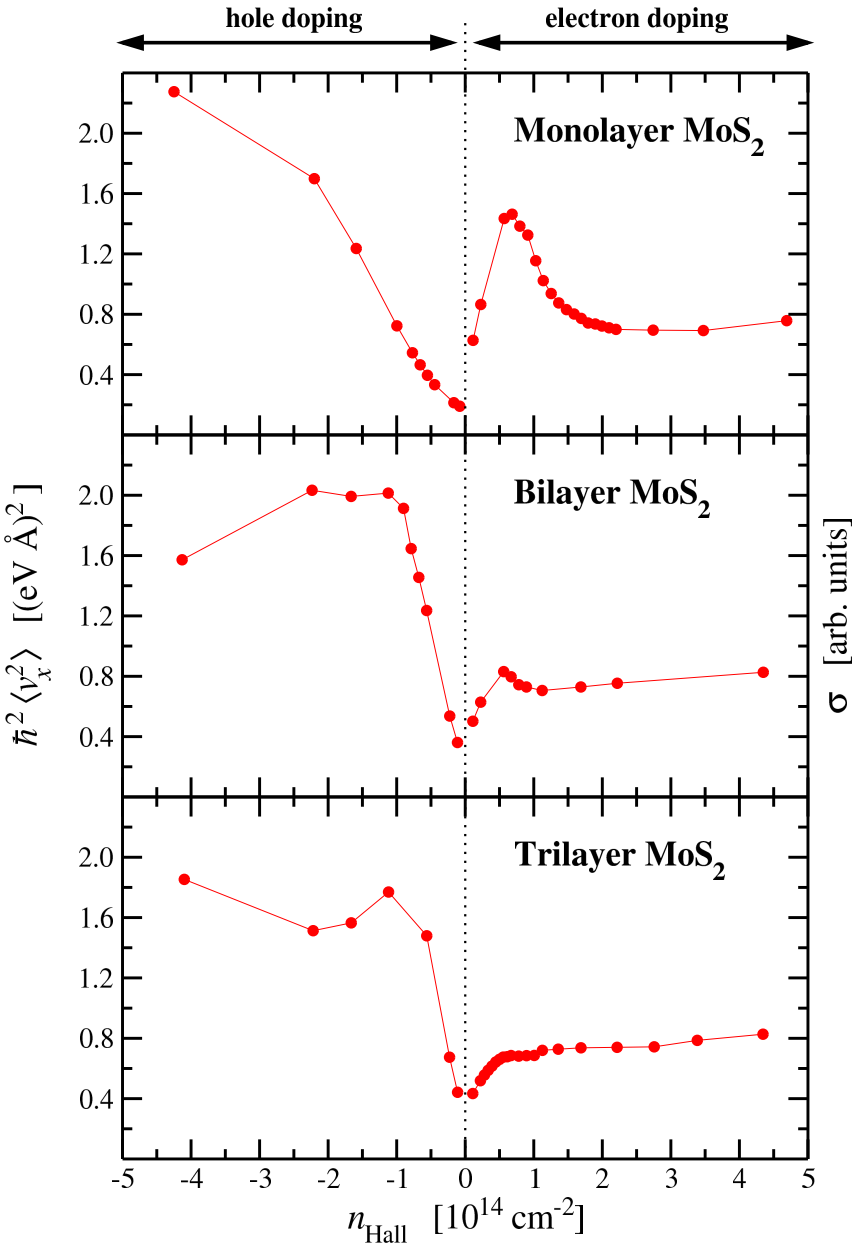

FIG. 11. Average squared velocity, $\langle v_x^2 \rangle$, for doping of MoS_2.

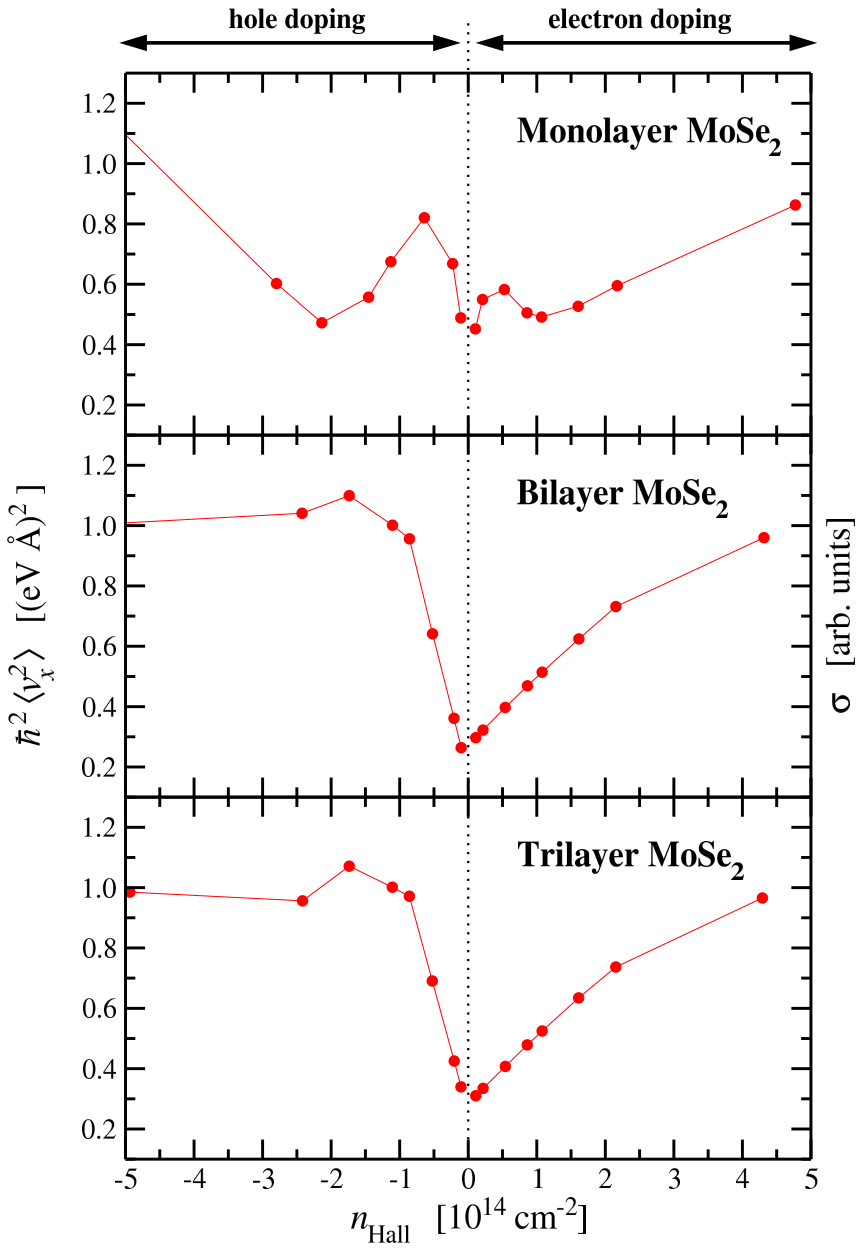

FIG. 12. Average squared velocity, $\langle v_x^2 \rangle$, for doping of $MoSe_2$.

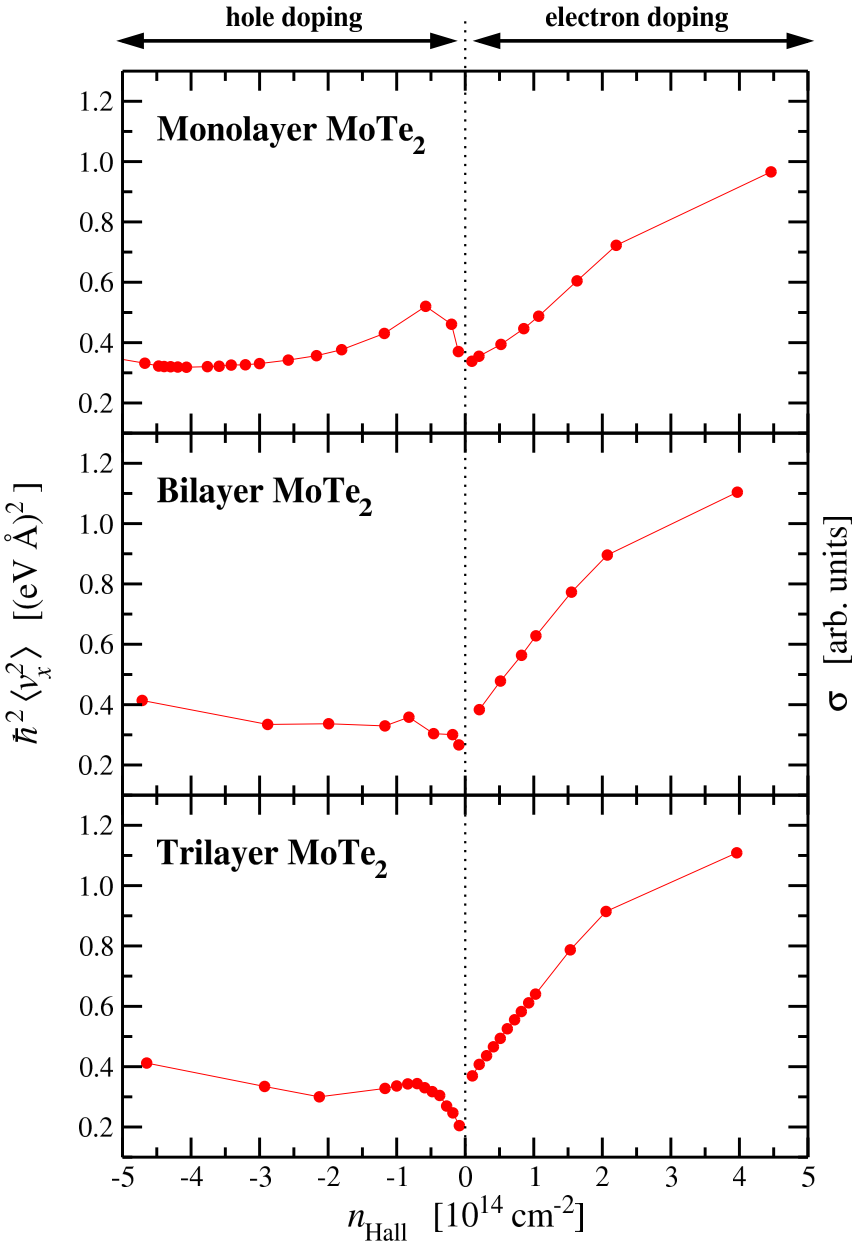

FIG. 13. Average squared velocity, $\langle v_x^2 \rangle$, for doping of $MoTe_2$.

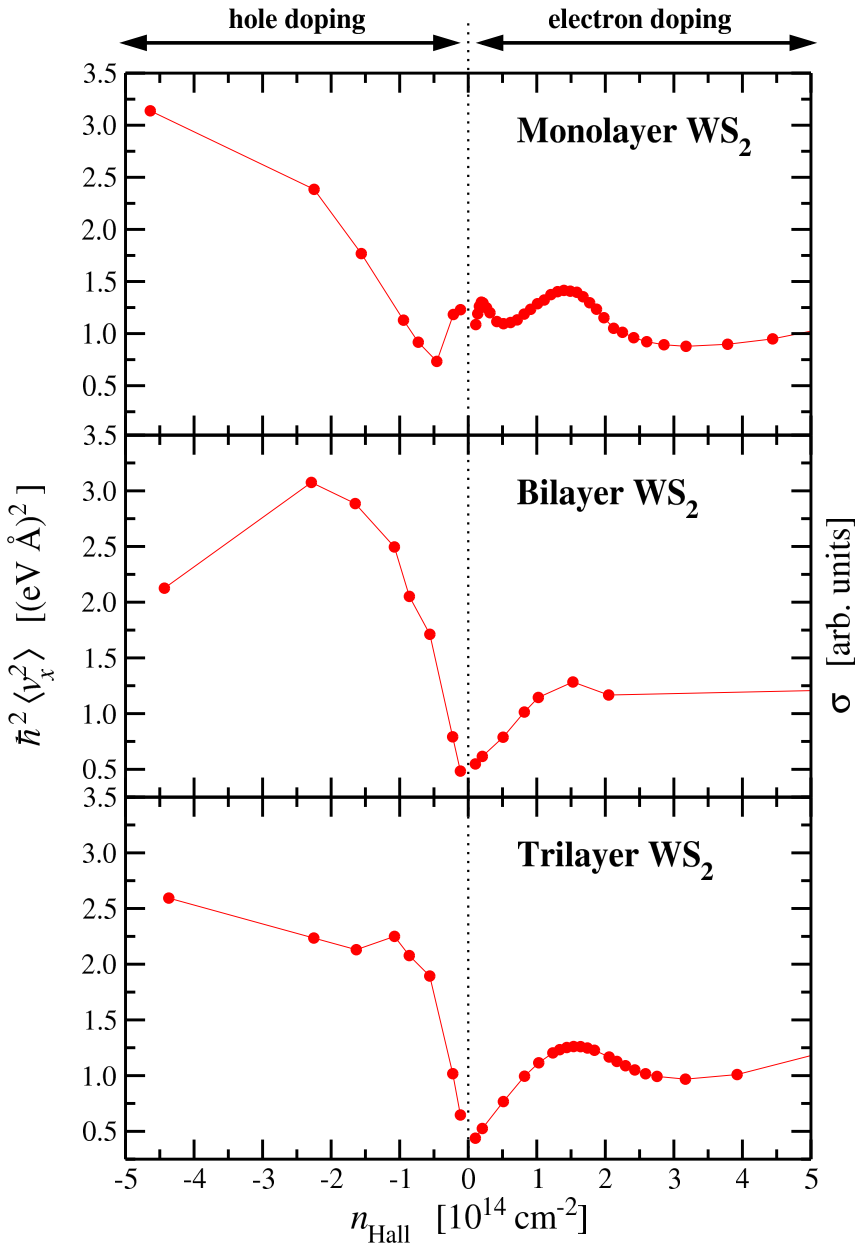

FIG. 14. Average squared velocity, $\langle v_x^2 \rangle$, for doping of WS_2.

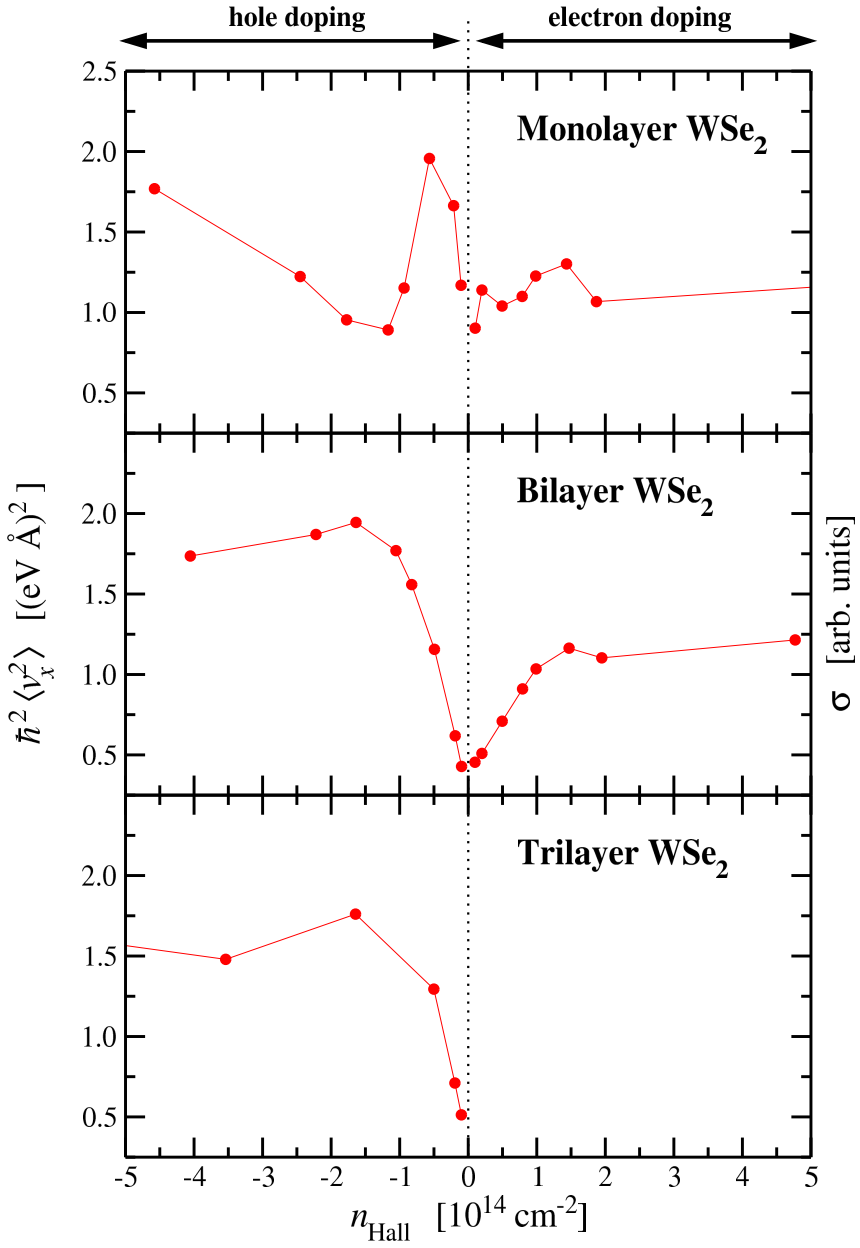

FIG. 15. Average squared velocity, $\langle v_x^2 \rangle$, for doping of WSe_2.

TABLE XI. Average squared velocity, $\langle v_x^2 \rangle$, for doping of MoS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and $\hbar^2\langle v_x^2 \rangle$ is given in $(\mathrm{eV\,\AA})^2$.

Monolayer		Bilayer		Trilayer	
n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$
-4.2491626	2.2754479	-4.1296552	1.5719507	-4.098818	1.8532922
-2.2011886	1.6990584	-2.2339244	2.0333336	-2.2187374	1.5134226
-1.5893042	1.2360298	-1.6642117	1.992077	-1.6633634	1.5649212
-0.99733892	0.72324514	-1.1231998	2.01411	-1.118947	1.769598
-0.76974118	0.54446013	-0.89985239	1.9130686	-0.5618741	1.4793742
-0.65771863	0.46481291	-0.7888849	1.6459781	-0.22901122	0.6743263
-0.55163215	0.39525363	-0.6777032	1.4556671	-0.1110224	0.44207673
-0.4460156	0.33295566	-0.56312938	1.235885		
-0.16556166	0.21338812	-0.22625942	0.53612364	0.10995963	0.43363351
-0.080191802	0.19008123	-0.11270142	0.36115747	0.22156061	0.51856175
				0.27967357	0.55647052
0.11447109	0.6268891	0.11152738	0.50147473	0.33361732	0.58717279
0.22717979	0.86475137	0.22604931	0.62819496	0.39049075	0.61529424
0.56806524	1.4343564	0.56093065	0.83096846	0.44608101	0.64267429
0.68428702	1.4629643	0.6705943	0.79649512	0.49989295	0.66027096
0.79699679	1.3836295	0.7809586	0.74409287	0.55459743	0.67503775
0.91326164	1.3251152	0.89273174	0.72920411	0.612537	0.67741895
1.0285618	1.1550485	1.1223905	0.70580008	0.66906237	0.68581123
1.1387553	1.0229258	1.6864759	0.72877135	0.7805717	0.68145415
1.2548959	0.93752688	2.2188961	0.75392708	0.89396019	0.68475058
1.3646634	0.87493645	4.3488299	0.82632362	1.0072688	0.68598131
1.4778319	0.83099943			1.1263014	0.71978556
1.588172	0.8015325			1.3575356	0.72769585
1.6921762	0.77224483			1.6882634	0.7364864
1.7924943	0.74209682			2.2153162	0.74007738
1.8970672	0.73531499			2.7577624	0.74340943
1.9946949	0.72154246			3.385373	0.78582198
2.0979988	0.71027629			4.3441106	0.82698872
2.200607	0.69946839				
2.7410158	0.69468993				
3.4741789	0.69188848				
4.6899383	0.75719196				

TABLE XII. $\langle v_x^2 \rangle$ for doping of $MoSe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and $\hbar^2\langle v_x^2 \rangle$ is given in $(\mathrm{eV\,\AA})^2$.

Monolayer		Bilayer		Trilayer	
n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$
4.7731017	0.86288947	4.3135928	0.96007884	4.2919296	0.96569286
2.1740007	0.59542128	2.1536538	0.73160784	2.1532276	0.73699188
1.6047773	0.52719115	1.614592	0.62457508	1.6118883	0.63445534
1.06965	0.49141846	1.0784851	0.51409804	1.0787673	0.52472434
0.85700705	0.50536504	0.86478195	0.46913589	0.86075675	0.47863702
0.52784856	0.5825211	0.53990246	0.3972134	0.54118178	0.40749303
0.20882683	0.54940094	0.21625638	0.32240791	0.21718596	0.33458563
0.10482951	0.45218913	0.10943795	0.29714484	0.10985212	0.31003202
-0.10919585	0.488635	-0.10345193	0.26393225	-0.10622988	0.33949884
-0.2266871	0.66835549	-0.2068659	0.36120123	-0.20377378	0.42535762
-0.64057209	0.82053139	-0.52061929	0.64147412	-0.52379019	0.69072405
-1.1283666	0.67480367	-0.85704697	0.95631031	-0.85834509	0.97157088
-1.4527003	0.55719403	-1.1047955	1.0011877	-1.1069769	1.0012983
-2.1359692	0.47220479	-1.7359182	1.0992678	-1.7362424	1.0710092
-2.7973089	0.60225652	-2.4247998	1.0408507	-2.4176947	0.95640298
-5.192778	1.1391835	-5.0129648	1.0088964	-4.9377152	0.98512106

TABLE XIII. $\langle v_x^2 \rangle$ for doping of $MoTe_2$. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and $\hbar^2\langle v_x^2 \rangle$ is given in $(\mathrm{eV\,\AA})^2$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$
4.4620591	0.96601517	3.9705544	1.1042605	3.9618465	1.1086758
2.2025426	0.72248281	2.0731326	0.89579471	2.0542661	0.91449735
1.6313633	0.60483701	1.549368	0.77281102	1.5328462	0.78725975
1.0716865	0.48749312	1.0309044	0.62801231	1.0251345	0.64057284
0.85378092	0.44615814	0.82200827	0.56344788	0.92619229	0.61168686
0.52184321	0.39398638	0.51422428	0.4781598	0.8181898	0.58265588
0.20057799	0.35485032	0.20624584	0.38324542	0.72017951	0.55532884
0.097547599	0.33822947			0.61406719	0.52553039
		-0.09308686	0.26634844	0.51177305	0.49364382
-0.099293354	0.37049488	-0.1835839	0.3004172	0.41117527	0.46575358
-0.19965373	0.46081495	-0.46162918	0.30394245	0.31200062	0.43636154
-0.57692017	0.52020406	-0.82214208	0.35841573	0.20405912	0.4074206
-1.1801887	0.43025635	-1.1718632	0.32952702	0.10362789	0.36933993
-1.8026589	0.37648186	-1.9935264	0.33675359		
-2.1701622	0.35657266	-2.8829782	0.33433944	-0.085827864	0.20441898
-2.5816873	0.3421077	-4.7128308	0.41387928	-0.17998372	0.24655275
-3.0018669	0.33051135			-0.27090748	0.26952713
-3.2069041	0.32665074			-0.37262262	0.30451684
-3.4136277	0.3254631			-0.48212991	0.31722208
-3.5902112	0.3216279			-0.59139557	0.33019701
-3.7614088	0.32022494			-0.7013484	0.34386735
-4.0672504	0.31849005			-0.83829488	0.34279531
-4.1935898	0.31905472			-0.99985758	0.33597815
-4.298634	0.31992905			-1.1696198	0.32799763
-4.3931009	0.32080924			-2.1292659	0.29999531
-4.4735689	0.32219712			-2.9264294	0.33443098
-4.6748095	0.33187226			-4.6471898	0.41188709
-6.9799483	0.4199339				

TABLE XIV. $\langle v_x^2 \rangle$ for doping of WS_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and $\hbar^2\langle v_x^2 \rangle$ is given in $(\mathrm{eV\,\AA})^2$.

Monolayer		Bilayer		Trilayer	
n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$
5.9451187	1.1499363	5.2540225	1.2093436	5.2034001	1.2116046
4.4418238	0.94859056	2.0490091	1.1664833	3.9235511	1.0093516
3.7841895	0.89711579	1.5269852	1.2835559	3.1687812	0.96801464
3.1775658	0.87781416	1.0226057	1.1452138	2.7548765	0.99289053
2.8561	0.89238646	0.81866269	1.0134903	2.5875534	1.0163955
2.6044336	0.92157705	0.50848075	0.78751976	2.4296378	1.050669
2.4141684	0.96053538	0.20564131	0.61530029	2.2947373	1.0884178
2.2500813	1.0118375	0.10373654	0.54816717	2.1691808	1.1271207
2.1217414	1.0503361			2.0553287	1.166963
1.9800159	1.1519045	-0.11360442	0.48344881	1.8418346	1.2274472
1.8708091	1.2335072	-0.22732088	0.79136891	1.7391726	1.2479591
1.7718938	1.295709	-0.56065269	1.711523	1.6389206	1.2600383
1.6762202	1.3529727	-0.85870253	2.0520457	1.5368319	1.2605919
1.5846173	1.3963308	-1.0767483	2.4961208	1.4373844	1.2519777
1.4892628	1.4069353	-1.6487975	2.8856825	1.3346483	1.2329513
1.395736	1.4144634	-2.2884839	3.0754539	1.233926	1.2039725
1.3021736	1.4016209	-4.4329284	2.1254837	1.0285453	1.1149667
1.2059799	1.3739843			0.82193897	0.99432584
1.1082159	1.3217205			0.5134167	0.76687997
1.0096871	1.2861241			0.20575059	0.52473306
0.90940289	1.2324733			0.10408891	0.4378139
0.81522236	1.1868726				
0.71454245	1.1311886			-0.11385782	0.64646707
0.61765518	1.1060551			-0.22574283	1.0176291
0.5136024	1.094466			-0.56095037	1.8941376
0.4172856	1.1148103			-0.8601742	2.0775605
0.31699533	1.2002724			-1.0760957	2.2500565
0.26755249	1.2468827			-1.6331629	2.1307131
0.21545743	1.2932226			-2.2530974	2.2346888
0.19181099	1.3009718			-4.3691497	2.5938833
0.16303181	1.2619401				
0.1381423	1.1906469				
0.11042201	1.0859813				
-0.11293672	1.2287663				
-0.21645275	1.1828296				
-0.45803433	0.73233022				
-0.72866793	0.91660927				
-0.94492107	1.1284819				
-1.5601135	1.7678314				
-2.2487039	2.3838756				
-4.6386124	3.1378683				

TABLE XV. $\langle v_x^2 \rangle$ for doping of WSe_2. The Hall charge, n_{Hall}, is given in $10^{14}\,\mathrm{cm}^{-2}$ (positive for electron doping, negative for hole doping), and $\hbar^2\langle v_x^2 \rangle$ is given in $(\mathrm{eV\,\AA})^2$.

Monolayer		**Bilayer**		**Trilayer**	
n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$	n_{Hall}	$\hbar^2\langle v_x^2 \rangle$
5.3796416	1.1678413	4.7701666	1.2145151	4.7387494	2.111284
1.8705484	1.0672591	1.9484388	1.1033448	1.9499477	1.9053643
1.4346005	1.3013285	1.4716749	1.163238	1.4735385	1.5712444
0.98360345	1.2259873	0.99029849	1.0346571	0.79438521	1.2405282
0.78776111	1.0993108	0.79288934	0.910204	0.49792702	1.0462165
0.49414791	1.0396303	0.49623851	0.70925169	0.20276075	0.61322831
0.20053258	1.1388843	0.19929835	0.50895018	0.10165173	0.34482837
0.10072038	0.90246373	0.098916827	0.45444384		
				-0.10069895	0.51290685
-0.10447814	1.1689722	-0.097819854	0.42854504	-0.19406515	0.71072744
-0.21338905	1.6636782	-0.19052331	0.61861327	-0.50087544	1.2944135
-0.56555008	1.9570158	-0.49230567	1.156185	-1.6441675	1.7606182
-0.93591402	1.1519317	-0.82473921	1.5585206	-3.5378885	1.4794016
-1.1686202	0.89161567	-1.0538261	1.7693235	-5.8117567	1.6129353
-1.774195	0.95403404	-1.6377766	1.9446001		
-2.4512037	1.2227923	-2.2216063	1.8699677		
-4.5769638	1.768884	-4.0546696	1.7358521		

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