

**Supporting Information**  
for  
**Microscopic contributions to the deviation from Amontons friction law**

Suresh Ravisankar<sup>\*1</sup>, Ravikant Kumar<sup>\*1</sup>, Antonio Cammarata<sup>1</sup>, Thilo Glatzel<sup>2</sup> and Tomas Polcar<sup>1</sup>

Address: <sup>1</sup>Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague 6, Czech Republic and <sup>2</sup>Department of Physics, University of Basel, 4056 Basel, Switzerland

Email: Suresh Ravisankar - ravissur@fel.cvut.cz; Ravikant Kumar - kumarra2@fel.cvut.cz

\* Corresponding author

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## Structural Information

The geometry of each hetrostructure used in the molecular dynamics simulations with a total number of 360 atoms (144 TM, 36 M, 72 X, 108 Si) is provided in what follows in POSCAR format.

Au/MoS<sub>2</sub>/Si

1.0

15.5672988892	0.0000000000	0.0000000000
0.0000000000	17.9267997742	0.0000000000
0.0000000000	0.0000000000	50.0000000000

Au	Mo	S	Si
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144	36	72	108
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Cartesian

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9.078979199	10.118999500	36.510199308
9.078979199	16.094600137	36.510199308
14.268078520	4.143399932	36.510199308
14.268078520	10.118999500	36.510199308
14.268078520	16.094600137	36.510199308

Au/MoSe<sub>2</sub>/Si

1.0

15.9442605972	0.0000000000	0.0000000000
0.0000000000	18.3540554047	0.0000000000
0.0000000000	0.0000000000	50.0000000000

Au	Mo	Se	Si
144	36	72	108

Cartesian

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0.0000000000	6.118018651	20.000000298
0.0000000000	12.236037301	20.000000298
5.314753691	0.0000000000	20.000000298
5.314753691	6.118018651	20.000000298
5.314753691	12.236037301	20.000000298
10.629507382	0.0000000000	20.000000298
10.629507382	6.118018651	20.000000298
10.629507382	12.236037301	20.000000298
5.185026843	6.001260705	26.669687033

5.185026843	12.119279356	26.669687033
5.185026843	18.237297459	26.669687033
10.499780534	6.001260705	26.669687033
10.499780534	12.119279356	26.669687033
10.499780534	18.237297459	26.669687033
15.814533749	6.001260705	26.669687033
15.814533749	12.119279356	26.669687033
15.814533749	18.237297459	26.669687033
0.000000000	3.059009325	20.000000298
0.000000000	9.177027702	20.000000298
0.000000000	15.295045806	20.000000298
5.314753691	3.059009325	20.000000298
5.314753691	9.177027702	20.000000298
5.314753691	15.295045806	20.000000298
10.629507382	3.059009325	20.000000298
10.629507382	9.177027702	20.000000298
10.629507382	15.295045806	20.000000298
5.185026843	2.942251380	26.669687033
5.185026843	9.060269757	26.669687033
5.185026843	15.178287860	26.669687033
10.499780534	2.942251380	26.669687033
10.499780534	9.060269757	26.669687033
10.499780534	15.178287860	26.669687033
15.814533749	2.942251380	26.669687033
15.814533749	9.060269757	26.669687033
15.814533749	15.178287860	26.669687033
1.726741453	6.070536335	22.249865532
1.726741453	12.188554985	22.249865532
1.726741453	18.306573089	22.249865532
7.041494787	6.070536335	22.249865532
7.041494787	12.188554985	22.249865532
7.041494787	18.306573089	22.249865532
12.356248478	6.070536335	22.249865532
12.356248478	12.188554985	22.249865532
12.356248478	18.306573089	22.249865532
1.726741453	3.011527557	22.249865532
1.726741453	9.129545934	22.249865532
1.726741453	15.247564584	22.249865532
7.041494787	3.011527557	22.249865532
7.041494787	9.129545934	22.249865532
7.041494787	15.247564584	22.249865532
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12.356248478	15.247564584	22.249865532
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3.452869453	12.155190571	24.451269209
3.452869453	18.273208675	24.451269209
8.767623381	6.037171921	24.451269209
8.767623381	12.155190571	24.451269209
8.767623381	18.273208675	24.451269209
14.082376597	6.037171921	24.451269209
14.082376597	12.155190571	24.451269209
14.082376597	18.273208675	24.451269209
3.452869453	2.978162595	24.451269209
3.452869453	9.096180973	24.451269209
3.452869453	15.214199076	24.451269209
8.767623381	2.978162595	24.451269209
8.767623381	9.096180973	24.451269209
8.767623381	15.214199076	24.451269209
14.082376597	2.978162595	24.451269209
14.082376597	9.096180973	24.451269209
14.082376597	15.214199076	24.451269209
4.386159060	1.483371096	22.249738872
4.386159060	7.601389473	22.249738872
4.386159060	13.719408124	22.249738872
9.700912751	1.483371096	22.249738872
9.700912751	7.601389473	22.249738872
9.700912751	13.719408124	22.249738872
15.015665967	1.483371096	22.249738872
15.015665967	7.601389473	22.249738872
15.015665967	13.719408124	22.249738872
4.386159060	4.542380695	22.249738872
4.386159060	10.660399619	22.249738872
4.386159060	16.778417722	22.249738872
9.700912751	4.542380695	22.249738872
9.700912751	10.660399619	22.249738872
9.700912751	16.778417722	22.249738872
15.015665967	4.542380695	22.249738872
15.015665967	10.660399619	22.249738872
15.015665967	16.778417722	22.249738872
0.796382790	1.444921420	24.454124272
0.796382790	7.562939661	24.454124272
0.796382790	13.680958858	24.454124272
6.111136303	1.444921420	24.454124272
6.111136303	7.562939661	24.454124272
6.111136303	13.680958858	24.454124272
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11.425889994	7.562939661	24.454124272
11.425889994	13.680958858	24.454124272
0.796382790	4.503931156	24.454124272

0.796382790	10.621949259	24.454124272
0.796382790	16.739968457	24.454124272
6.111136303	4.503931156	24.454124272
6.111136303	10.621949259	24.454124272
6.111136303	16.739968457	24.454124272
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11.425889994	10.621949259	24.454124272
11.425889994	16.739968457	24.454124272
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2.657376845	7.647522903	20.000000298
2.657376845	13.765541553	20.000000298
7.972130299	1.529504663	20.000000298
7.972130299	7.647522903	20.000000298
7.972130299	13.765541553	20.000000298
13.286883514	1.529504663	20.000000298
13.286883514	7.647522903	20.000000298
13.286883514	13.765541553	20.000000298
2.531148718	1.412257705	26.669946313
2.531148718	7.530275945	26.669946313
2.531148718	13.648294596	26.669946313
7.845902172	1.412257705	26.669946313
7.845902172	7.530275945	26.669946313
7.845902172	13.648294596	26.669946313
13.160655862	1.412257705	26.669946313
13.160655862	7.530275945	26.669946313
13.160655862	13.648294596	26.669946313
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2.657376845	10.706533049	20.000000298
2.657376845	16.824551152	20.000000298
7.972130299	4.588514398	20.000000298
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13.286883514	10.706533049	20.000000298
13.286883514	16.824551152	20.000000298
2.531148718	4.471267167	26.669946313
2.531148718	10.589286091	26.669946313
2.531148718	16.707304195	26.669946313
7.845902172	4.471267167	26.669946313
7.845902172	10.589286091	26.669946313
7.845902172	16.707304195	26.669946313
13.160655862	4.471267167	26.669946313
13.160655862	10.589286091	26.669946313
13.160655862	16.707304195	26.669946313
0.720179648	1.334453490	31.018465757

0.720179648	7.452472140	31.018465757
0.720179648	13.570490244	31.018465757
6.034933279	1.334453490	31.018465757
6.034933279	7.452472140	31.018465757
6.034933279	13.570490244	31.018465757
11.349686970	1.334453490	31.018465757
11.349686970	7.452472140	31.018465757
11.349686970	13.570490244	31.018465757
0.720179648	4.393462815	31.018465757
0.720179648	10.511481739	31.018465757
0.720179648	16.629499843	31.018465757
6.034933279	4.393462815	31.018465757
6.034933279	10.511481739	31.018465757
6.034933279	16.629499843	31.018465757
11.349686970	4.393462815	31.018465757
11.349686970	10.511481739	31.018465757
11.349686970	16.629499843	31.018465757
3.377824671	5.922980469	31.018307805
3.377824671	12.040999119	31.018307805
3.377824671	18.159017223	31.018307805
8.692577886	5.922980469	31.018307805
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8.692577886	18.159017223	31.018307805
14.007332052	5.922980469	31.018307805
14.007332052	12.040999119	31.018307805
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3.377824671	8.981990067	31.018307805
3.377824671	15.100008718	31.018307805
8.692577886	2.863971417	31.018307805
8.692577886	8.981990067	31.018307805
8.692577886	15.100008718	31.018307805
14.007332052	2.863971417	31.018307805
14.007332052	8.981990067	31.018307805
14.007332052	15.100008718	31.018307805
2.489290940	1.332780647	32.792428136
2.489290940	7.450798887	32.792428136
2.489290940	13.568817538	32.792428136
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7.804044393	13.568817538	32.792428136
13.118797609	1.332780647	32.792428136
13.118797609	7.450798887	32.792428136
13.118797609	13.568817538	32.792428136
2.489290940	4.391790109	32.792428136

2.489290940	10.509809033	32.792428136
2.489290940	16.627827136	32.792428136
7.804044393	4.391790109	32.792428136
7.804044393	10.509809033	32.792428136
7.804044393	16.627827136	32.792428136
13.118797609	4.391790109	32.792428136
13.118797609	10.509809033	32.792428136
13.118797609	16.627827136	32.792428136
5.146511928	5.921592199	32.792788744
5.146511928	12.039610850	32.792788744
5.146511928	18.157628953	32.792788744
10.461265619	5.921592199	32.792788744
10.461265619	12.039610850	32.792788744
10.461265619	18.157628953	32.792788744
15.776018834	5.921592199	32.792788744
15.776018834	12.039610850	32.792788744
15.776018834	18.157628953	32.792788744
5.146511928	2.862582874	32.792788744
5.146511928	8.980601251	32.792788744
5.146511928	15.098619355	32.792788744
10.461265619	2.862582874	32.792788744
10.461265619	8.980601251	32.792788744
10.461265619	15.098619355	32.792788744
15.776018834	2.862582874	32.792788744
15.776018834	8.980601251	32.792788744
15.776018834	15.098619355	32.792788744
2.493253195	1.336985386	29.265865684
2.493253195	7.455003626	29.265865684
2.493253195	13.573022824	29.265865684
7.808006886	1.336985386	29.265865684
7.808006886	7.455003626	29.265865684
7.808006886	13.573022824	29.265865684
13.122760577	1.336985386	29.265865684
13.122760577	7.455003626	29.265865684
13.122760577	13.573022824	29.265865684
2.493253195	4.395994848	29.265865684
2.493253195	10.514013225	29.265865684
2.493253195	16.632031328	29.265865684
7.808006886	4.395994848	29.265865684
7.808006886	10.514013225	29.265865684
7.808006886	16.632031328	29.265865684
13.122760577	4.395994848	29.265865684
13.122760577	10.514013225	29.265865684
13.122760577	16.632031328	29.265865684
5.150610796	5.925518518	29.265716672

5.150610796	12.043537169	29.265716672
5.150610796	18.161555273	29.265716672
10.465364487	5.925518518	29.265716672
10.465364487	12.043537169	29.265716672
10.465364487	18.161555273	29.265716672
15.780117702	5.925518518	29.265716672
15.780117702	12.043537169	29.265716672
15.780117702	18.161555273	29.265716672
5.150610796	2.866509740	29.265716672
5.150610796	8.984528117	29.265716672
5.150610796	15.102546768	29.265716672
10.465364487	2.866509740	29.265716672
10.465364487	8.984528117	29.265716672
10.465364487	15.102546768	29.265716672
15.780117702	2.866509740	29.265716672
15.780117702	8.984528117	29.265716672
15.780117702	15.102546768	29.265716672
0.440924002	1.211381598	35.891878605
0.440924002	7.329400249	35.891878605
0.440924002	13.447418900	35.891878605
5.755677574	1.211381598	35.891878605
5.755677574	7.329400249	35.891878605
5.755677574	13.447418900	35.891878605
11.070430790	1.211381598	35.891878605
11.070430790	7.329400249	35.891878605
11.070430790	13.447418900	35.891878605
3.098300729	2.719712554	35.891494155
3.098300729	8.837730931	35.891494155
3.098300729	14.955749035	35.891494155
8.413054657	2.719712554	35.891494155
8.413054657	8.837730931	35.891494155
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13.727807873	14.955749035	35.891494155
0.440924002	4.270391197	35.891878605
0.440924002	10.388409301	35.891878605
0.440924002	16.506428498	35.891878605
5.755677574	4.270391197	35.891878605
5.755677574	10.388409301	35.891878605
5.755677574	16.506428498	35.891878605
11.070430790	4.270391197	35.891878605
11.070430790	10.388409301	35.891878605
11.070430790	16.506428498	35.891878605
3.098300729	5.778721879	35.891494155



3.098300729	11.896740530	35.891494155
3.098300729	18.014758633	35.891494155
8.413054657	5.778721879	35.891494155
8.413054657	11.896740530	35.891494155
8.413054657	18.014758633	35.891494155
13.727807873	5.778721879	35.891494155
13.727807873	11.896740530	35.891494155
13.727807873	18.014758633	35.891494155
1.326716324	5.792836499	37.640830874
1.326716324	11.910855149	37.640830874
1.326716324	18.028873253	37.640830874
6.641469777	5.792836499	37.640830874
6.641469777	11.910855149	37.640830874
6.641469777	18.028873253	37.640830874
11.956223468	5.792836499	37.640830874
11.956223468	11.910855149	37.640830874
11.956223468	18.028873253	37.640830874
3.984093169	1.183149898	37.640309334
3.984093169	7.301168275	37.640309334
3.984093169	13.419186378	37.640309334
9.298846385	1.183149898	37.640309334
9.298846385	7.301168275	37.640309334
9.298846385	13.419186378	37.640309334
14.613600551	1.183149898	37.640309334
14.613600551	7.301168275	37.640309334
14.613600551	13.419186378	37.640309334
1.326716324	2.733827994	37.640830874
1.326716324	8.851846645	37.640830874
1.326716324	14.969864748	37.640830874
6.641469777	2.733827994	37.640830874
6.641469777	8.851846645	37.640830874
6.641469777	14.969864748	37.640830874
11.956223468	2.733827994	37.640830874
11.956223468	8.851846645	37.640830874
11.956223468	14.969864748	37.640830874
3.984093169	4.242158949	37.640309334
3.984093169	10.360177874	37.640309334
3.984093169	16.478195977	37.640309334
9.298846385	4.242158949	37.640309334
9.298846385	10.360177874	37.640309334
9.298846385	16.478195977	37.640309334
14.613600551	4.242158949	37.640309334
14.613600551	10.360177874	37.640309334
14.613600551	16.478195977	37.640309334
1.326716324	5.792836499	40.030124784

1.326716324	11.910855149	40.030124784
1.326716324	18.028873253	40.030124784
6.641469777	5.792836499	40.030124784
6.641469777	11.910855149	40.030124784
6.641469777	18.028873253	40.030124784
11.956223468	5.792836499	40.030124784
11.956223468	11.910855149	40.030124784
11.956223468	18.028873253	40.030124784
3.984093169	1.183149898	40.029674768
3.984093169	7.301168275	40.029674768
3.984093169	13.419186378	40.029674768
9.298846385	1.183149898	40.029674768
9.298846385	7.301168275	40.029674768
9.298846385	13.419186378	40.029674768
14.613600551	1.183149898	40.029674768
14.613600551	7.301168275	40.029674768
14.613600551	13.419186378	40.029674768
1.326716324	2.733827994	40.030124784
1.326716324	8.851846645	40.030124784
1.326716324	14.969864748	40.030124784
6.641469777	2.733827994	40.030124784
6.641469777	8.851846645	40.030124784
6.641469777	14.969864748	40.030124784
11.956223468	2.733827994	40.030124784
11.956223468	8.851846645	40.030124784
11.956223468	14.969864748	40.030124784
3.984093169	4.242158949	40.029674768
3.984093169	10.360177874	40.029674768
3.984093169	16.478195977	40.029674768
9.298846385	4.242158949	40.029674768
9.298846385	10.360177874	40.029674768
9.298846385	16.478195977	40.029674768
14.613600551	4.242158949	40.029674768
14.613600551	10.360177874	40.029674768
14.613600551	16.478195977	40.029674768

Au/WS2/Si

1.0

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0.0000000000	17.9489860535	0.0000000000
0.0000000000	0.0000000000	50.0000000000

Au	W	S	Si
144	36	72	108

Cartesian

0.0000000000	0.0000000000	20.000000298
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0.000000000	5.982999809	20.000000298
0.000000000	11.965999618	20.000000298
5.220340120	0.000000000	20.000000298
5.220340120	5.982999809	20.000000298
5.220340120	11.965999618	20.000000298
10.440699843	0.000000000	20.000000298
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Au/WSe2/Si

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Au	W	Se	Si
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Cartesian

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Ag/MoS2/Si

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Ag	Mo	S	Si
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Ag/MoSe2/Si

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Ag	Mo	Se	Si
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Cartesian

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Ag	W	Se	Si
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Cartesian

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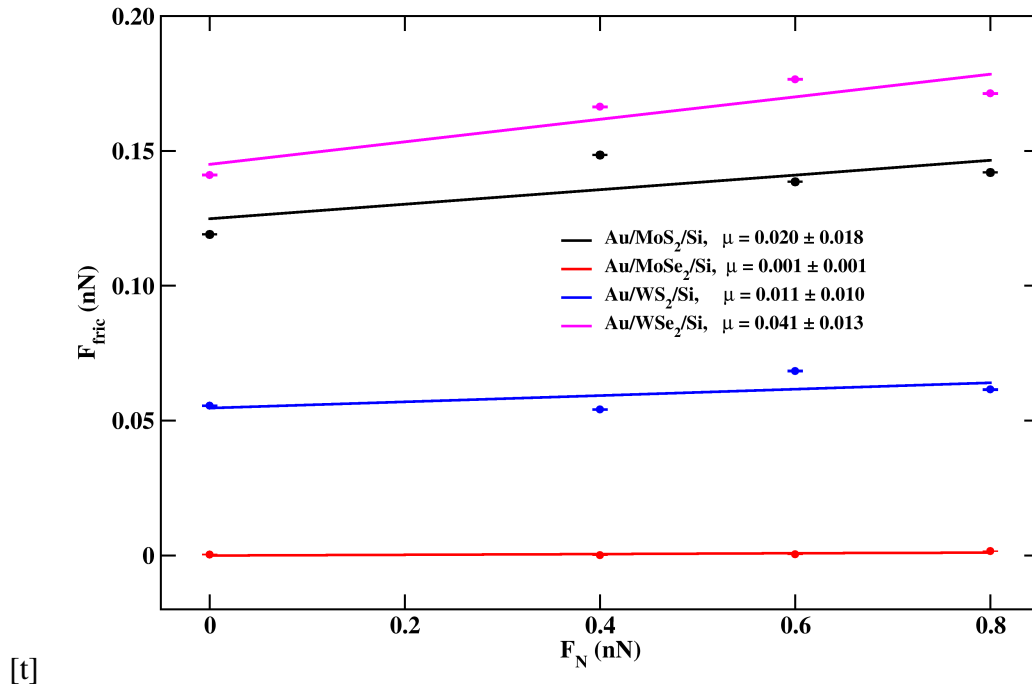


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## Frictional Properties

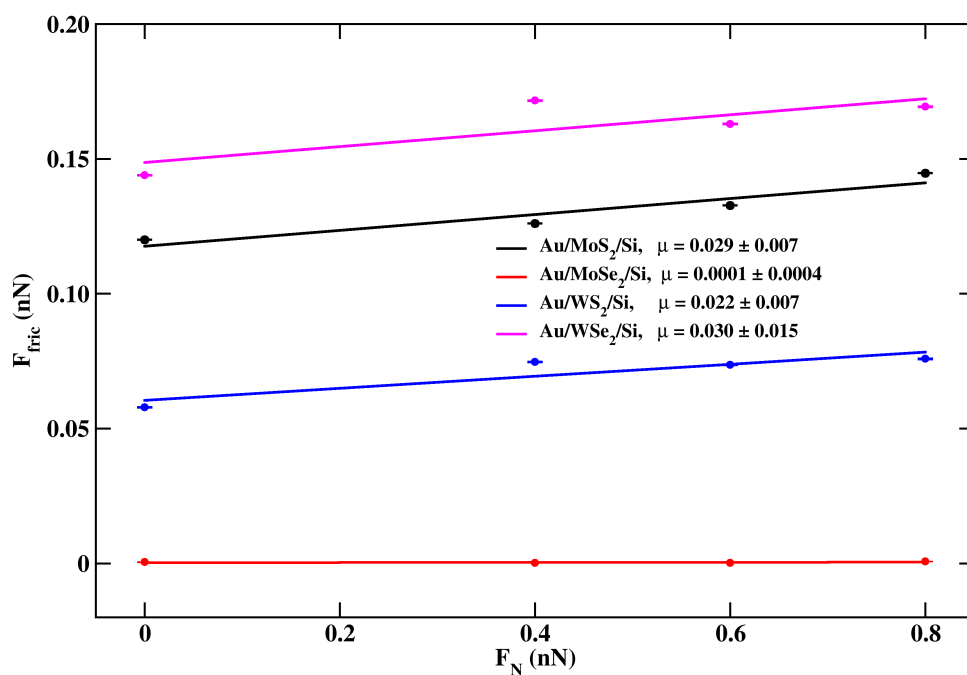


**Figure S1:**  $\mu$  using linear fit function on average friction force as a function of load for all the systems with a tip velocity of 3 m/s.

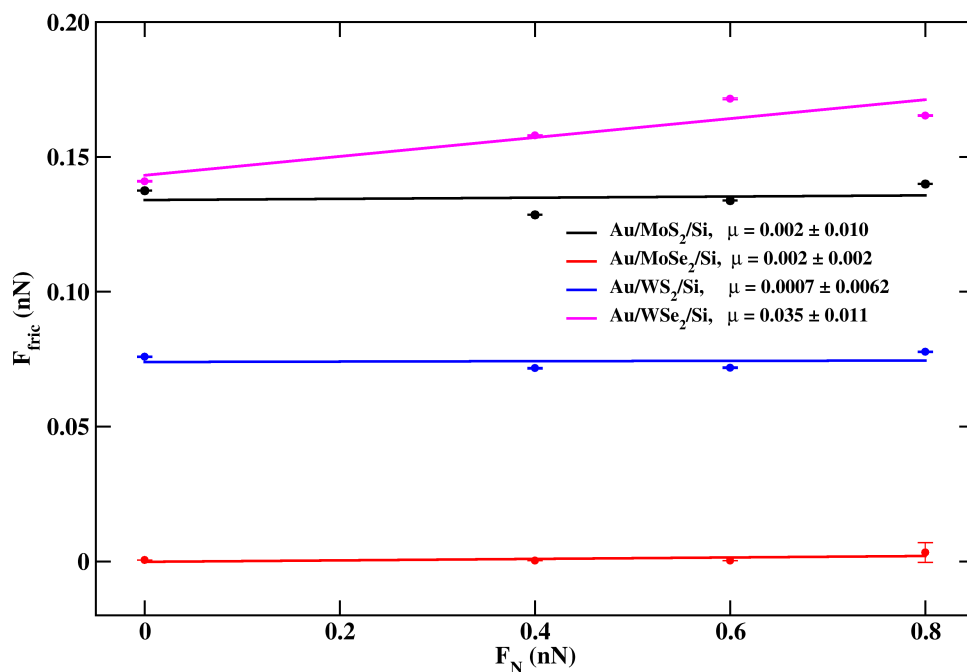
The Figure S1, Figure S2 and Figure S3 shows friction force as a function of normal load for four Au/MX<sub>2</sub>/Si systems except Au/MoS<sub>2</sub>/Si which is presented in the main manuscript, with linear fits used to extract the coefficient of friction  $\mu$ . Most of the systems exhibit nonmonotonic nature with loads and extraction of  $\mu$  from a linear fit results in large errors. This same trend is observed in Ag/MX<sub>2</sub>/Si systems as shown in Figure S6, Figure S7, Figure S8 and Figure S9.

The friction force profile for the Au/MoSe<sub>2</sub>/Si system is shown in Figure S4. In this case, both lateral slip and zigzag behaviour are suppressed and the tip moves along  $y$ -direction. This is also observed in the Fourier transform (FT) spectra of Au/MoSe<sub>2</sub>/Si where the second and third peaks, representing the lateral and zig-zag motions, are absent (Figure S5).

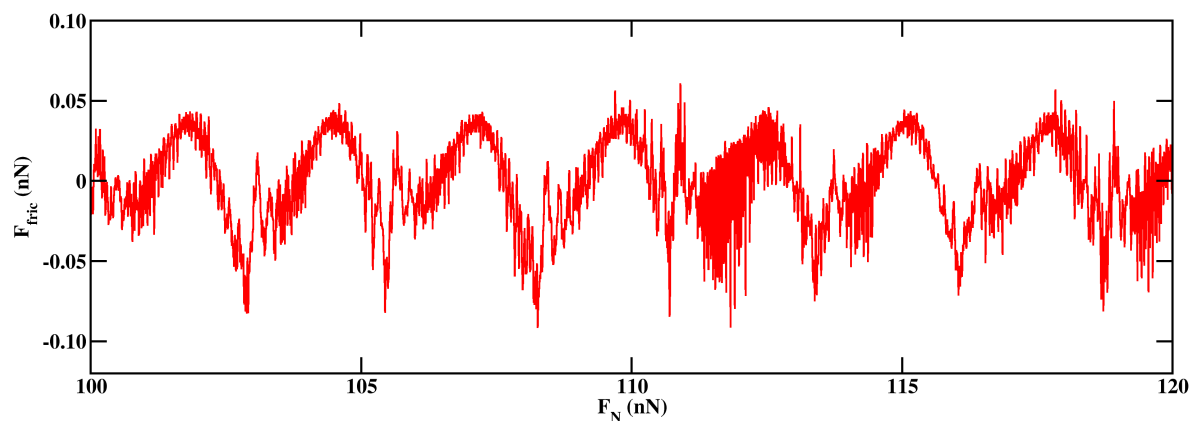
Figure S10 shows the spatial Fourier transform of the frictional force in the Ag/MX<sub>2</sub>/Si and Au/MX<sub>2</sub>/Si systems. In the Au/WSe<sub>2</sub>/Si case, the first peak dominates than the Ag/WSe<sub>2</sub>/Si system which leads to higher frictional force.



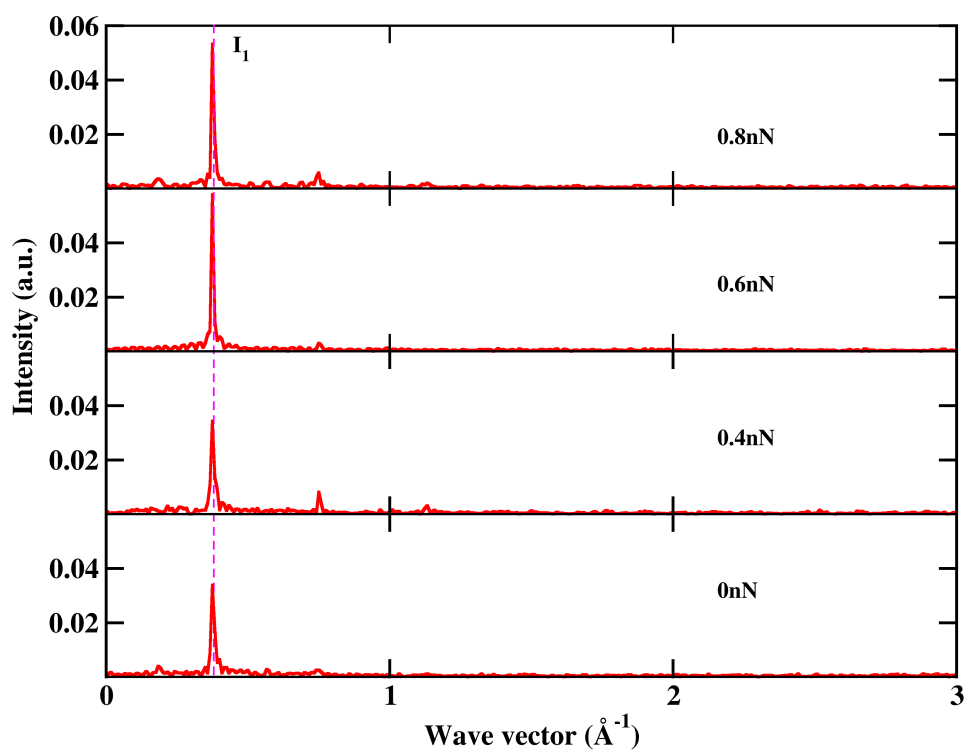
**Figure S2:**  $\mu$  using linear fit function on average friction force as a function of load for all the systems with a tip velocity of 4 m/s.



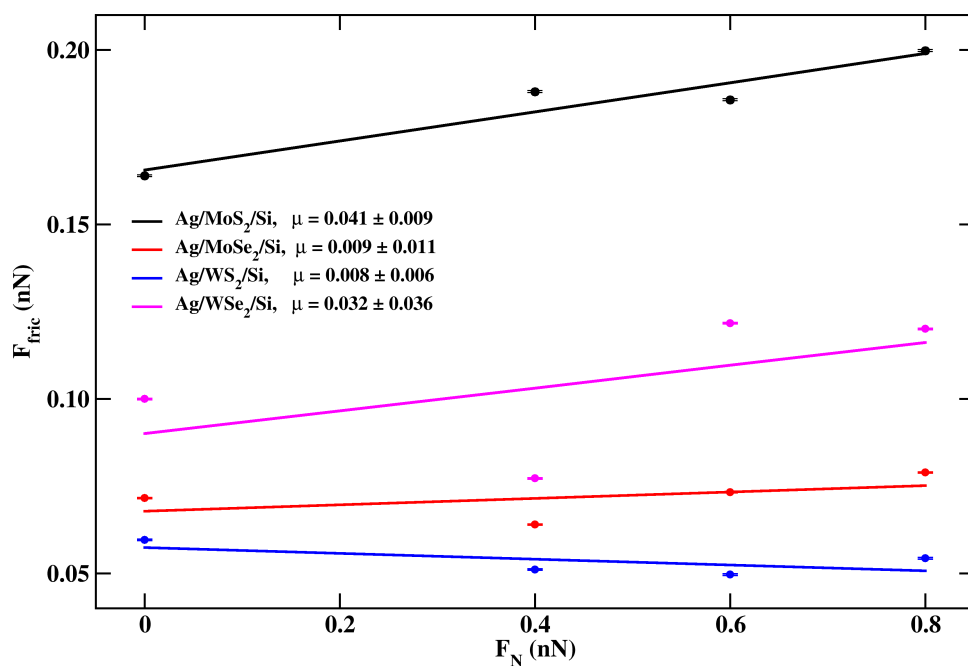
**Figure S3:**  $\mu$  using linear fit function on average friction force as a function of load for all the systems with a tip velocity of 5 m/s.



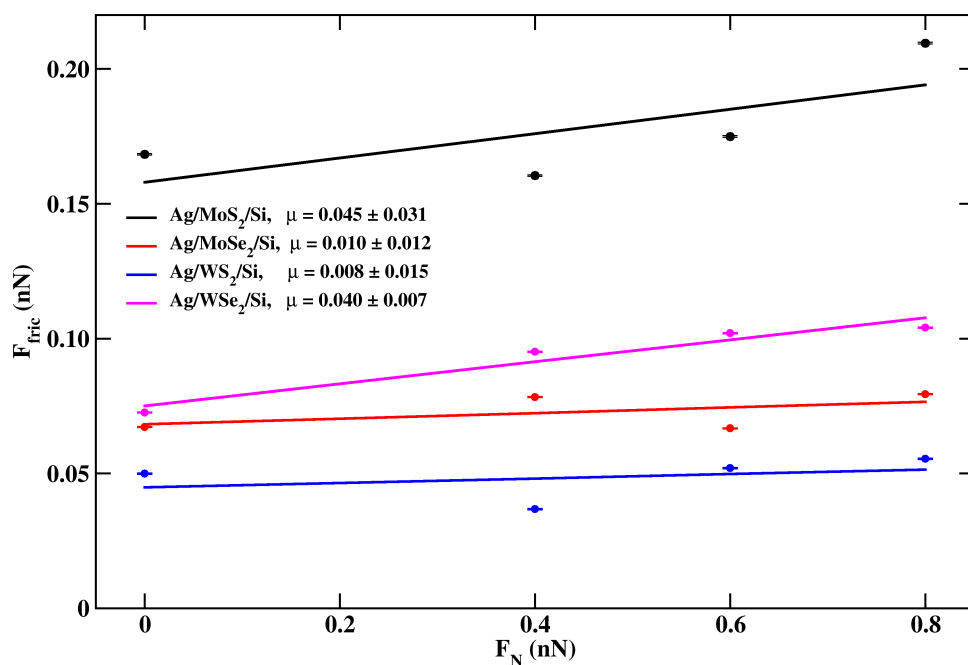
**Figure S4:** Friction force profile of Au/MoSe<sub>2</sub>/Si where tip moving with velocity 2 m/s for load of 0 nN.



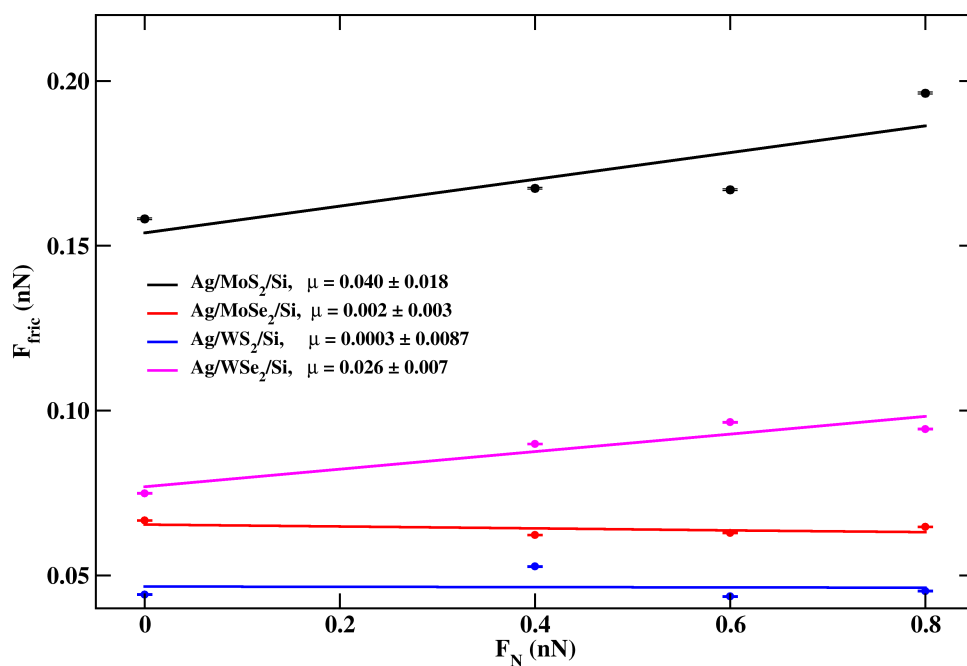
**Figure S5:** Spatial Fourier transform of Au/MoSe<sub>2</sub>/Si with varying loads at velocity 2 m/s.



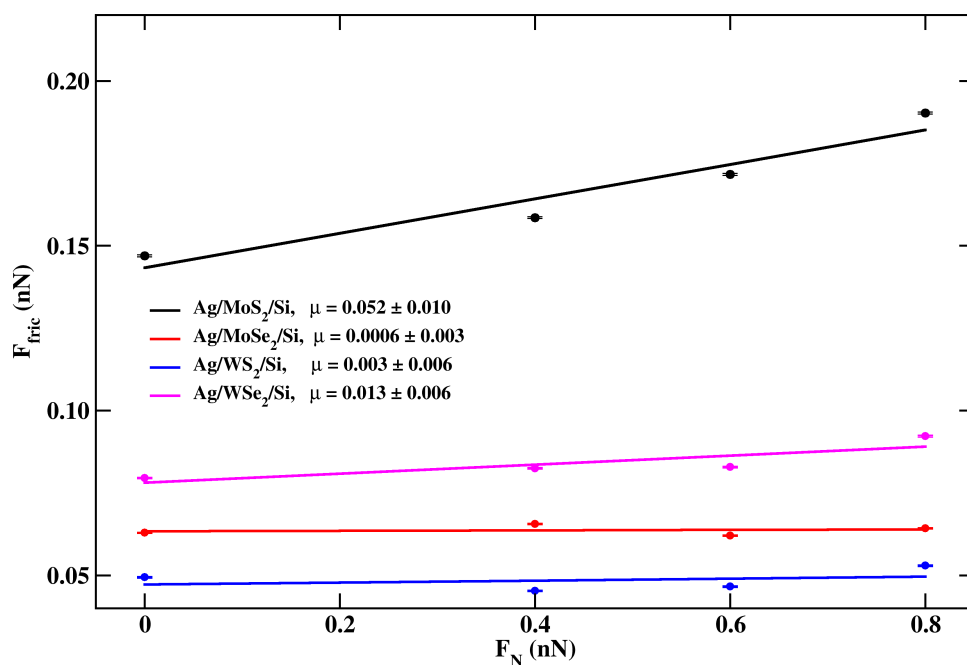
**Figure S6:**  $\mu$  extracted from a linear fit on the average friction force as a function of load with a tip velocity of 2 m/s.



**Figure S7:**  $\mu$  extracted from a linear fit function on the average friction force as a function of load with a tip velocity of 3 m/s.

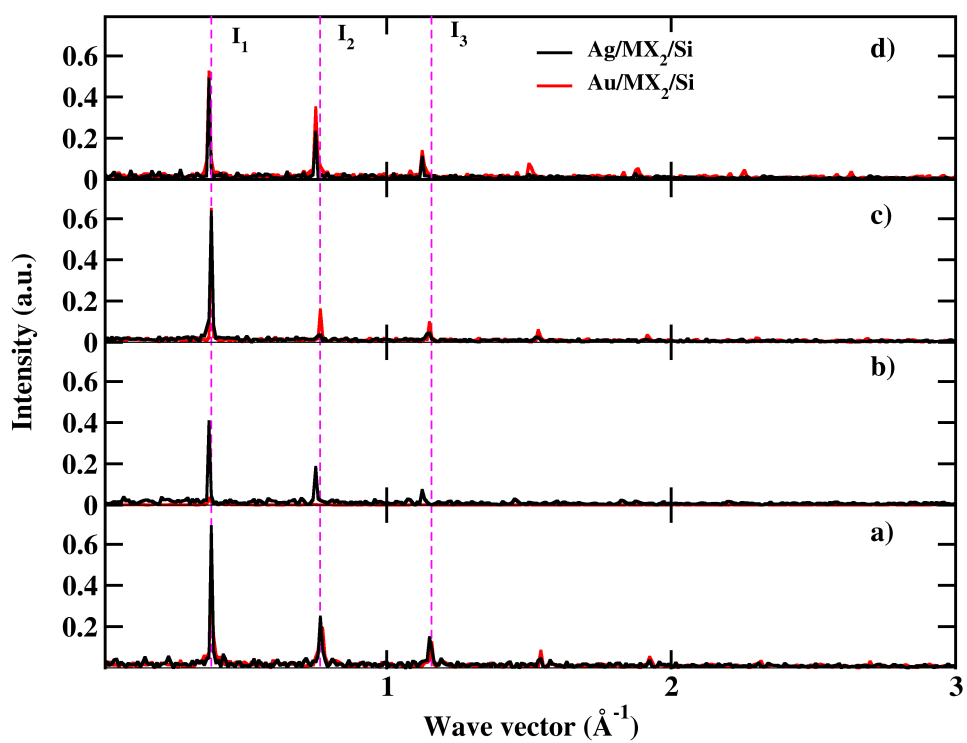


**Figure S8:**  $\mu$  extracted from a linear fit function on the average friction force as a function of load with a tip velocity of 4 m/s.



**Figure S9:**  $\mu$  extracted from a linear fit function on the average friction force as a function of load with a tip velocity of 5 m/s.





**Figure S10:** Spatial Fourier transform of friction force with monolayer a) MoS<sub>2</sub>, b) MoSe<sub>2</sub>, c) WS<sub>2</sub> and d) WSe<sub>2</sub> at different substrates.