Supplementary Information

Tuning Electronic and Magnetic Properties of Silicene with Magnetic Superhalogens

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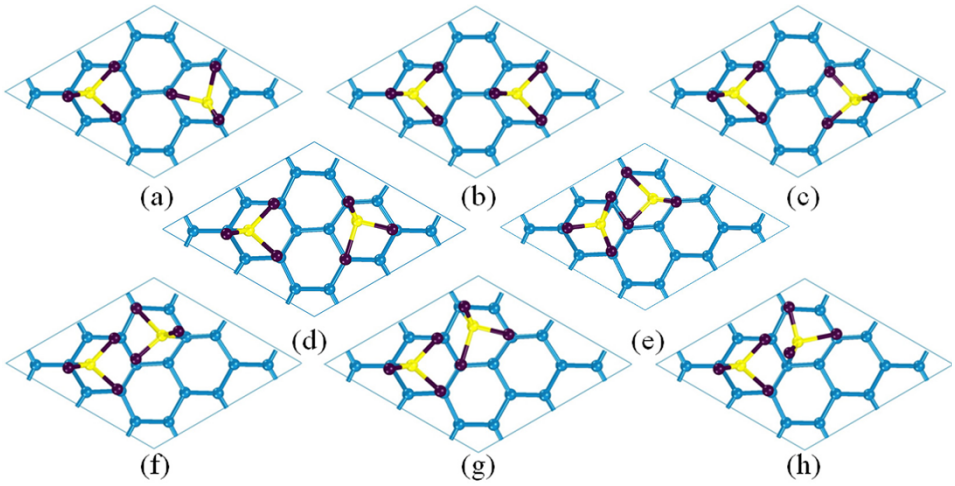

Fig. S1 Eight initial configurations of the $2MnCl_3$-adsorbed silicene where the two superhalogens on the same side of silicene.

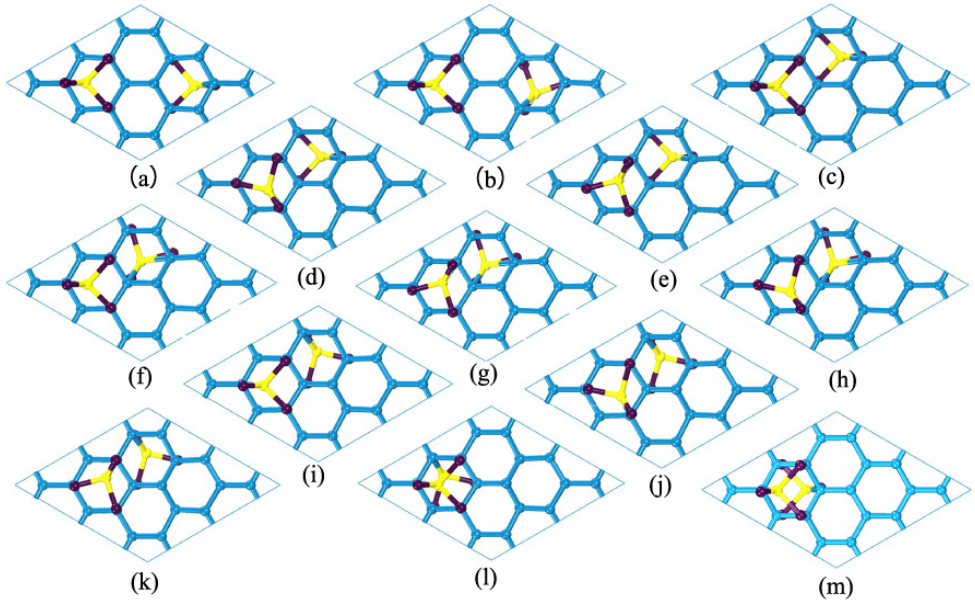

Fig. S2 Thirteen initial configurations of the $2MnCl_3$-adsorbed silicene where the two superhalogens on the opposite sides of silicene.

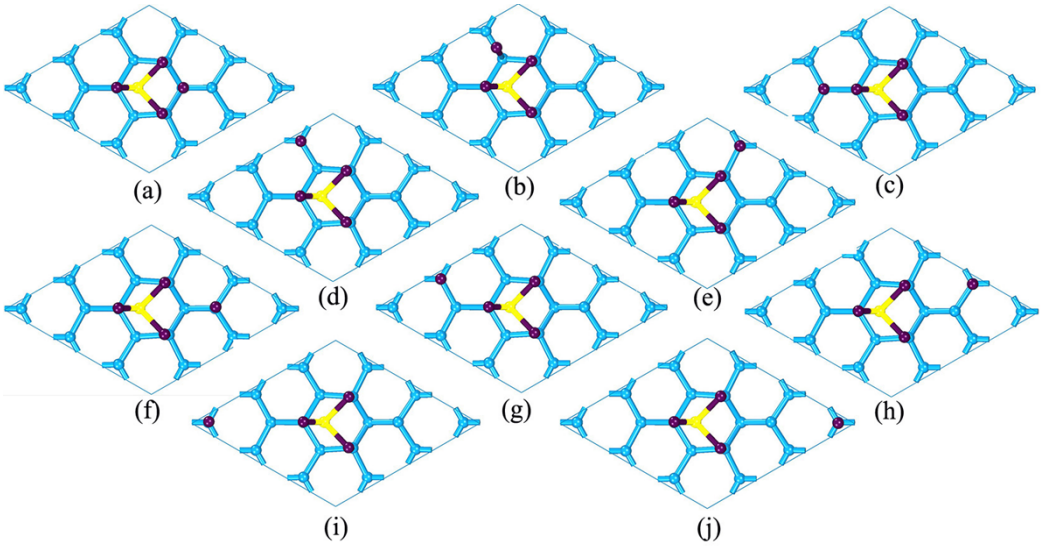

Fig. S3 Ten initial configurations of the $MnCl_3$ and Cl co-adsorbed silicene where both the Cl atom and $MnCl_3$ molecule are on the same side of silicene.

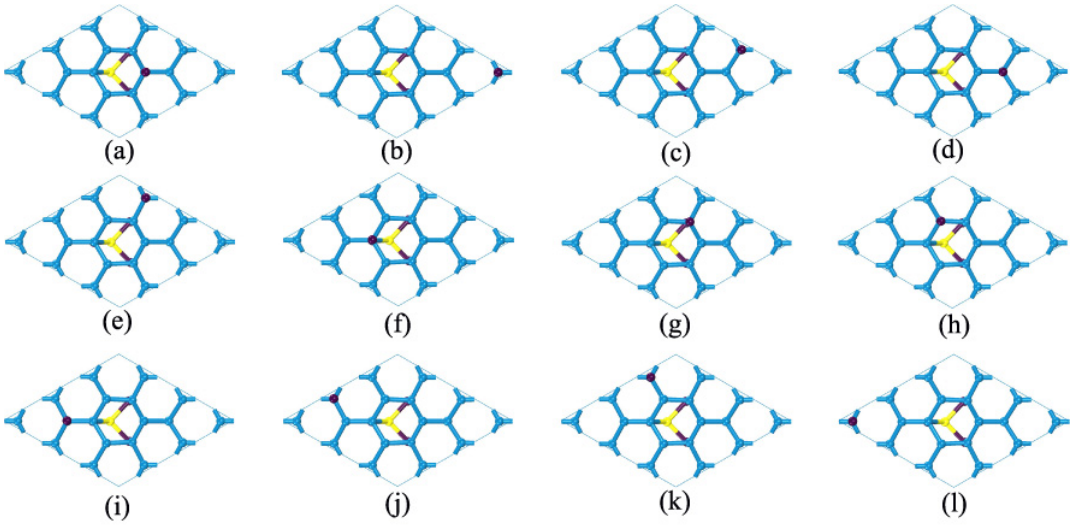

Fig. S4 Twelve initial configurations of $MnCl_3$ and Cl co-adsorbed silicene where the Cl atom and $MnCl_3$ are on the opposite sites of silicene.

Coordinates of the lowest energy configurations for each adsorption species and coverage in the 3x3 supercell.

1) Modulation with one $MnCl_3$ molecule:

a = b = 11.67 A, c = 15 A, $\alpha = \beta = 90$ $\gamma = 120°$

Si	Si1	0.2853	0.0639	0.5548
Si	Si2	0.4062	0.2889	0.5954
Si	Si3	0.6220	0.0639	0.5564
Si	Si4	0.7247	0.2877	0.5797
Si	Si5	0.9515	0.0606	0.5659
Si	Si6	0.2851	0.3926	0.5543
Si	Si7	0.3944	0.6176	0.5602
Si	Si8	0.6161	0.3961	0.5285
Si	Si9	0.7240	0.6060	0.5953
Si	Si10	0.9483	0.3903	0.5559

Si	Si11	0.2813	0.7312	0.5496
Si	Si12	0.6194	0.7269	0.5554
Si	Si13	0.9488	0.7272	0.5542
Si	Si14	0.3968	0.9525	0.5784
Si	Si15	0.7281	0.9496	0.5904
Si	Si16	0.0647	0.9476	0.5873
Si	Si17	0.0626	0.2842	0.5898
Si	Si18	0.0599	0.6155	0.5779
Cl	Cl19	0.3982	0.3083	0.7428
Cl	Cl20	0.7067	0.6139	0.7430
Cl	Cl21	0.3966	0.6220	0.8126
Mn	Mn22	0.4699	0.5467	0.7053

2) Modulation with $MnCl_3$ in high coverage

Two $MnCl_3$ adsorbed on the same side of silicene sheet:

a = b = 11.67 A, c = 15 A, $\alpha = \beta = 90$ $\gamma = 120°$

Si	Si1	0.0964	0.2221	0.5689
Si	Si2	0.2258	0.4504	0.6010
Si	Si3	0.4330	0.2237	0.5577
Si	Si4	0.5502	0.4531	0.5888
Si	Si5	0.7640	0.2231	0.5759
Si	Si6	0.1024	0.5586	0.5772
Si	Si7	0.2052	0.7756	0.5403
Si	Si8	0.4322	0.5505	0.5270
Si	Si9	0.5365	0.7604	0.5944
Si	Si10	0.7615	0.5440	0.5220
Si	Si11	0.0902	0.8893	0.5453
Si	Si12	0.4266	0.8775	0.5577
Si	Si13	0.7634	0.8856	0.5591

Si	Si14	0.2067	0.1074	0.5811
Si	Si15	0.5402	0.1076	0.5594
Si	Si16	0.8745	0.1051	0.5961
Si	Si17	0.8697	0.4543	0.6038
Si	Si18	0.8672	0.7642	0.5691
Cl	Cl19	0.2239	0.4709	0.7465
Cl	Cl20	0.5118	0.7791	0.7400
Cl	Cl21	0.1828	0.7616	0.8084
Cl	Cl22	0.8503	0.4388	0.7492
Cl	Cl23	0.5439	0.4262	0.7371
Cl	Cl24	0.5549	0.1210	0.8209
Mn	Mn25	0.2759	0.7090	0.7016
Mn	Mn26	0.6148	0.2588	0.7083

Two $MnCl_3$ adsorbed on the opposite sides of silicene sheet:

a = b = 11.67 A, c = 15 A, $\alpha = \beta = 90$ $\gamma = 120°$

Si	Si1	0.0939	0.2151	0.5550
Si	Si2	0.2071	0.4397	0.5846
Si	Si3	0.4310	0.2177	0.5419
Si	Si4	0.5429	0.4357	0.5967
Si	Si5	0.7582	0.2190	0.5437
Si	Si6	0.0958	0.5500	0.5581
Si	Si7	0.2066	0.7713	0.5854
Si	Si8	0.4301	0.5481	0.5627
Si	Si9	0.5383	0.7710	0.5850
Si	Si10	0.7597	0.5453	0.5399
Si	Si11	0.0944	0.8835	0.5536
Si	Si12	0.4285	0.8834	0.5607
Si	Si13	0.7626	0.8836	0.5546

Si	Si14	0.2052	0.1048	0.5810
Si	Si15	0.5412	0.1092	0.5998
Si	Si16	0.8710	0.1065	0.5772
Si	Si17	0.8703	0.4372	0.5978
Si	Si18	0.8725	0.7713	0.5784
Cl	Cl19	0.5245	0.1370	0.7435
Cl	Cl20	0.8469	0.4563	0.7415
Cl	Cl21	0.5536	0.4485	0.8742
Cl	Cl22	0.4553	0.1995	0.3982
Cl	Cl23	0.7757	0.5166	0.3962
Cl	Cl24	0.7510	0.2019	0.2686
Mn	Mn25	0.6019	0.3834	0.7502
Mn	Mn26	0.6999	0.2704	0.3899

3) Hybrid modulation with $MnCl_3$ and Cl

The Cl and $MnCl_3$ co-adsorbed silicene with Cl atom on the same side of $MnCl_3$.

a = b = 11.67 A, c = 15 A, $\alpha = \beta = 90$ $\gamma = 120°$

Si	Si1	0.2860	0.0647	0.5585
Si	Si2	0.4116	0.2923	0.5937
Si	Si3	0.6222	0.0662	0.5590
Si	Si4	0.7253	0.2915	0.6022
Si	Si5	0.9511	0.0620	0.5660
Si	Si6	0.2874	0.3932	0.5523
Si	Si7	0.3952	0.6178	0.5538
Si	Si8	0.6209	0.3919	0.5248
Si	Si9	0.7213	0.6016	0.5932
Si	Si10	0.9481	0.3915	0.5540
Si	Si11	0.2826	0.7317	0.5442
Si	Si12	0.6198	0.7261	0.5539

Si	Si13	0.9487	0.7273	0.5572
Si	Si14	0.3975	0.9521	0.5752
Si	Si15	0.7259	0.9490	0.5871
Si	Si16	0.0638	0.9492	0.5852
Si	Si17	0.0645	0.2877	0.5851
Si	Si18	0.0616	0.6159	0.5728
Cl	Cl19	0.3991	0.3097	0.7402
Cl	Cl20	0.7052	0.6137	0.7398
Cl	Cl21	0.3966	0.6213	0.8124
Cl	Cl22	0.7350	0.2970	0.7423
Mn	Mn23	0.4679	0.5479	0.7030

The Cl and $MnCl_3$ co-adsorbed silicene with Cl on the opposite sides of $MnCl_3$.

a = b = 11.67 A, c = 15 A, $\alpha = \beta = 90$ $\gamma = 120°$

Si	Si1	0.2821	0.0607	0.5503
Si	Si2	0.3931	0.2843	0.5916
Si	Si3	0.6201	0.0627	0.5589
Si	Si4	0.7303	0.2821	0.5913
Si	Si5	0.9487	0.0631	0.5580
Si	Si6	0.2825	0.3911	0.5368
Si	Si7	0.3963	0.6139	0.5687
Si	Si8	0.6184	0.3936	0.5450
Si	Si9	0.7288	0.6188	0.5917
Si	Si10	0.9495	0.3922	0.5584
Si	Si11	0.2835	0.7291	0.5552
Si	Si12	0.6198	0.7288	0.5399
Si	Si13	0.9521	0.7305	0.5496
Si	Si14	0.3941	0.9516	0.5806
Si	Si15	0.7266	0.9463	0.5862
Si	Si16	0.0618	0.9507	0.5814

Si	Si17	0.0660	0.2855	0.5850
Si	Si18	0.0609	0.6183	0.5800
Cl	Cl19	0.4088	0.3057	0.7375
Cl	Cl20	0.7097	0.6042	0.7381
Cl	Cl21	0.3950	0.6223	0.8162
Cl	Cl22	0.6111	0.4011	0.4058
Mn	Mn23	0.4725	0.5485	0.7116