Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Impact of van der Waal's interaction in the hybrid bilayer of Silicene/SiC

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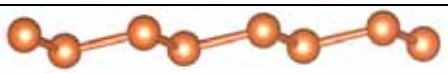
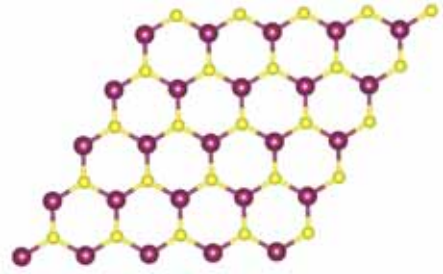
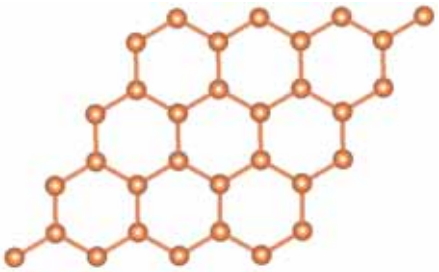
SiC sheet	Silicene
	
Side View	
	
Top View	

Figure S1: Top and side views of silicene and SiC monolayer sheets. (*Si of SiC sheet: purple, C: yellow, Si of Silicene sheet: Orange*)

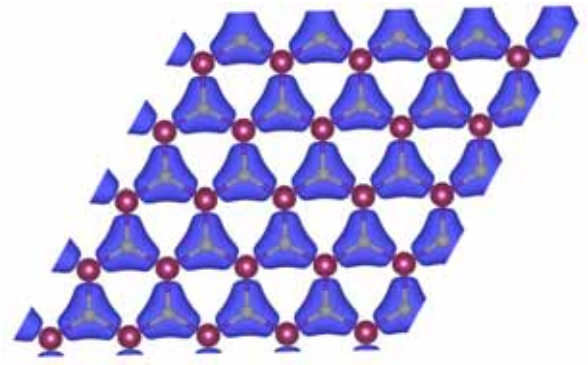


Figure S2: Isosurface of the pristine SiC sheet. The contour value is set as 1/4th of maximum.

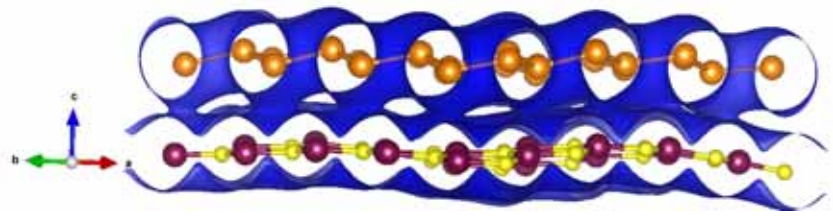


Figure S3: The charge density contours of silicene/SiC bilayer. The contour value is 0.01 electron/bohr^3.

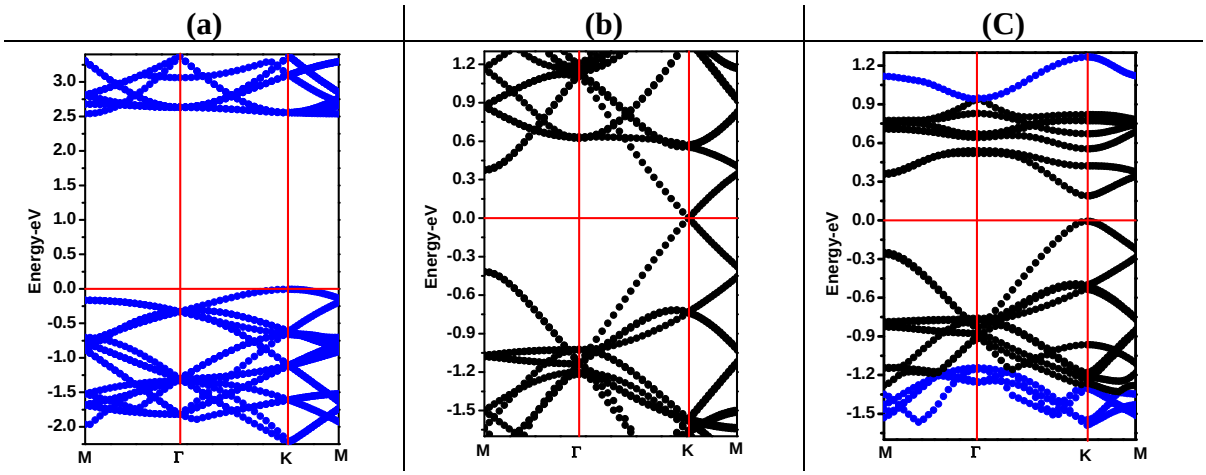


Figure S4: Band structure of (a) pristine SiC sheet (b) pristine silicene and (c) silicene/SiC hybrid bilayer.

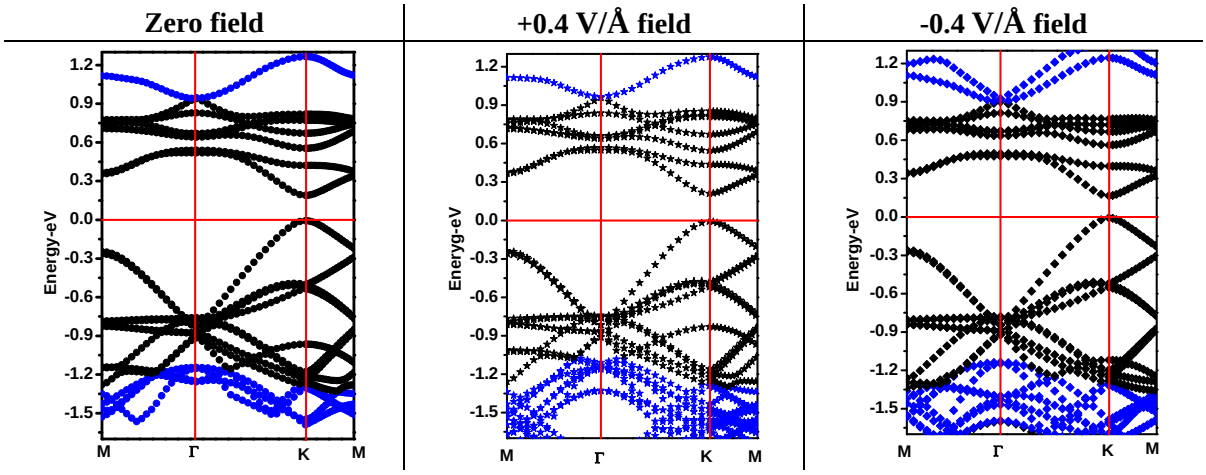


Figure S5: Band structure of silicene/SiC bilayer under the influence of electric field.

Initial configuration (coordinates) of Silicene –SiC bilayer

C	-4.41797	11.06666	7.272291
C	-2.91705	8.468179	7.25588
C	-1.41808	11.06569	7.263953
C	-1.41633	5.868821	7.267689
C	0.082633	3.272123	7.272291
C	0.082727	8.467103	7.261121
C	1.581676	5.868884	7.268875
C	1.583314	11.06556	7.263173
C	1.583548	0.673639	7.25588
C	3.082318	8.468054	7.256309
C	3.082521	3.271148	7.263953
C	4.583093	5.868595	7.254562
C	4.583233	11.06666	7.272291
C	4.583327	0.672563	7.261121
C	6.083914	3.271016	7.263173
C	6.084148	8.468179	7.25588
C	7.582918	0.673514	7.256309
C	7.583121	11.06569	7.263953
C	7.584868	5.868821	7.267689
C	9.083833	3.272123	7.272291
C	9.083927	8.467103	7.261121
C	10.58288	5.868884	7.268875
C	10.58475	0.673639	7.25588
C	12.08372	3.271148	7.263953
C	13.58453	0.672563	7.261121
Si	-5.91848	11.93187	7.267775
Si	-4.41792	9.332989	7.253431
Si	-2.91802	6.735799	7.249336
Si	-2.91749	11.93186	7.269171
Si	-1.41788	4.137331	7.267775
Si	-1.41788	9.333207	7.252892
Si	0.082594	6.735932	7.263625
Si	0.08268	1.538449	7.253431
Si	0.082696	11.93231	7.252674
Si	1.583111	4.137315	7.269171
Si	1.583314	9.333184	7.252916
Si	3.082724	1.538667	7.252892
Si	3.082724	11.93187	7.267775
Si	3.083356	6.735838	7.250498
Si	4.58328	9.332989	7.253431
Si	4.583296	4.137767	7.252674
Si	6.083181	6.735799	7.249336
Si	6.083711	11.93186	7.269171
Si	6.083914	1.538644	7.252916
Si	7.583324	4.137331	7.267775
Si	7.583324	9.333207	7.252892

Si	9.083794	6.735932	7.263625
Si	9.08388	1.538449	7.253431
Si	10.58431	4.137315	7.269171
Si	12.08392	1.538667	7.252892
Si	1.92368	1.11085	10.45332
Si	-0.00022	4.44287	10.4533
Si	-1.92406	7.77533	10.45466
Si	5.77129	1.11099	10.45211
Si	3.84741	4.44295	10.45188
Si	1.92354	7.77549	10.45333
Si	9.61845	1.11092	10.45199
Si	7.69463	4.44286	10.45199
Si	5.77075	7.77533	10.45362
Si	-0.00009	2.22147	9.98387
Si	-1.92398	5.55393	9.98538
Si	-3.84781	8.88588	9.98544
Si	3.84712	2.22128	9.98406
Si	1.92323	5.55384	9.98553
Si	-0.00063	8.88581	9.98538
Si	7.69469	2.22146	9.98274
Si	5.77088	5.55394	9.98418
Si	3.84698	8.88592	9.98407
Si	13.46568	1.11085	10.45332
Si	11.54178	4.44287	10.4533
Si	9.61794	7.77533	10.45466
Si	11.54191	2.22147	9.98387
Si	9.61802	5.55393	9.98538
Si	7.69419	8.88588	9.98544
Si	-3.84632	11.10685	10.45332
Si	0.00129	11.10699	10.45211
Si	3.84845	11.10692	10.45199
Si	-5.77009	12.21747	9.98387
Si	-1.92288	12.21728	9.98406
Si	1.92469	12.21746	9.98274
Si	7.69568	11.10685	10.45332
Si	5.77191	12.21747	9.98387

Final optimized configuration (coordinates) of Silicene –SiC bilayer

C	-4.61893	11.20314	7.5684
C	-3.08898	8.53368	7.74172
C	-1.54946	11.20049	7.9196
C	-1.54778	5.86471	7.84055
C	-0.00688	3.19701	7.69906
C	-0.00689	8.53433	7.83644
C	1.53396	5.86473	7.84071
C	1.53576	11.20046	7.91738
C	1.54063	0.53778	7.5493
C	3.07543	8.53355	7.74019
C	3.07029	3.196	7.94218
C	4.61244	5.86964	7.98905
C	4.60534	11.20305	7.56496
C	4.60269	0.52952	8.01823
C	6.14384	3.20138	8.28746
C	6.15263	8.52544	7.63052
C	7.68969	0.52637	8.25462
C	7.68982	11.19625	7.34874
C	7.68972	5.87732	8.09702
C	9.2355	3.20143	8.28596
C	9.22676	8.52545	7.63053
C	10.76675	5.86963	7.9875
C	10.77646	0.52943	8.01458
C	12.30886	3.19605	7.93842
C	13.83851	0.53795	7.54567
Si	-6.16585	12.08705	7.49637
Si	-4.63298	9.42604	7.64961
Si	-3.09462	6.75631	7.86922
Si	-3.0992	12.08654	7.8752
Si	-1.54837	4.07851	7.83574
Si	-1.5527	9.42858	7.83571
Si	-0.00687	6.75351	7.8275
Si	-0.00691	1.41459	7.60037
Si	-0.00671	12.08528	8.09797
Si	1.53459	4.0786	7.83726
Si	1.53913	9.42846	7.83434
Si	3.06157	1.41178	7.88009
Si	3.08556	12.08644	7.87162
Si	3.08088	6.75623	7.86947
Si	4.61932	9.42601	7.64802
Si	4.60576	4.08864	8.15134
Si	6.1549	6.76986	7.95862
Si	6.15222	12.08703	7.49394
Si	6.13717	1.41392	8.28849
Si	7.68963	4.10075	8.33053
Si	7.68972	9.42453	7.5479

Si	9.2244	6.76984	7.95808
Si	9.24226	1.41388	8.2861
Si	10.77343	4.08859	8.14847
Si	12.31739	1.41183	7.87602
Si	1.90766	1.11168	11.47513
Si	-0.00543	4.44532	11.61713
Si	-1.9262	7.77775	11.63914
Si	5.75263	1.10015	11.85454
Si	3.82455	4.4521	11.7351
Si	1.91537	7.77781	11.63851
Si	9.62948	1.10015	11.85191
Si	7.69123	4.45837	11.90269
Si	5.75997	7.78968	11.54513
Si	-0.00524	2.25807	10.97389
Si	-1.93362	5.5578	11.09636
Si	-3.82722	8.86662	11.00276
Si	3.87682	2.23366	11.21912
Si	1.92297	5.55766	11.09699
Si	-0.00554	8.88538	11.07605
Si	7.69084	2.22609	11.43758
Si	5.77788	5.52705	11.26464
Si	3.81655	8.86635	11.002
Si	13.47445	1.11175	11.47315
Si	11.55768	4.45194	11.73327
Si	9.62243	7.78969	11.54538
Si	11.50528	2.23366	11.21633
Si	9.60429	5.52713	11.26362
Si	7.69125	8.84394	10.95403
Si	-3.8576	11.09889	11.49844
Si	-0.0054	11.08952	11.70229
Si	3.84667	11.09892	11.49591
Si	-5.74448	12.23397	10.9173
Si	-1.90624	12.24264	11.20246
Si	1.89513	12.24244	11.20056
Si	7.69104	11.10801	11.24664
Si	5.73384	12.23402	10.91588