Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

"Y"-shaped BP/PbS/PbSe nano-devices based on silicon carbide nanoribbons

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S1. Calculate methods of electron-transport properties.

Here the most of electron-transport properties of the structure are handled by the non-equilibrium Green function formalism:

$$G(E) = (ES - H - \Sigma_1 - \Sigma_2)^{-1} \quad (1)$$

A recursive method[1] is utilized to process the self-energy matrices $\Sigma_{1,2}$ which are used to describe the effect of the regions of source and drain electrodes. After the model is chemically bonded to electrode contacts, its energy levels are broadened due to the hybridization with the delocalized wave functions in contacts. Thus, the self-energy matrices $\Sigma_{1,2}$ of contacts are used to account for their effect on the "Y"-shaped model with broadening functions defined as $\Gamma_{1,2} = i(\Sigma_{1,2} - \Sigma_{1,2}^{+})$.[2]

The formula for the density matrix ρ is used as follows:

$$\rho = \frac{1}{2\pi}\int_{-\infty}^{\infty} dE(f_1 G\Gamma_1 G^{+} + f_2 G\Gamma_2 G^{+}) \quad (2)$$

G and G^{+} represent the Green's function matrices reflected from the left and right electrodes to the central scattering region.

The transmission T represents the electron transmission probability:

$$T(E,V) = trace(\Gamma_1 G\Gamma_2 G^{+}) \quad (4)$$

The effect of gate voltage is taken into account by shifting the scattering region of the Hamiltonian with Vg. Details of such a theoretical method can be found in Refs.[3]

Table S1. Structure file of tri-SiC (atom, corresponding x, y and z Cartesian coordinates in Å.

H	19.751962662	10.046944618	0.829033434
H	19.751962662	10.046944618	7.019402504
H	29.616277695	26.758432388	0.767166555
H	29.616277695	26.758432388	6.957532883
H	10.133015633	26.739244461	0.695370734
H	10.133015633	26.739244461	6.885736942
H	19.751962662	10.046944618	3.924221992
H	29.616277695	26.758432388	3.862352610
H	10.133015633	26.739244461	3.790556669
Si	19.652181625	11.540089607	0.824370205

Si	19.652181625	11.540089607	7.014740467
Si	19.336135864	16.825511932	0.820551991
Si	19.336135864	16.825511932	7.010915279
Si	23.741312027	23.409229279	0.765552759
Si	23.741312027	23.409229279	6.955916882
Si	28.331363678	26.004650116	0.766133130
Si	28.331363678	26.004650116	6.956501961
Si	15.799848557	23.023534775	0.706190228
Si	15.799848557	23.023534775	6.896554470
Si	11.393211365	25.940557480	0.700916946
Si	11.393211365	25.940557480	6.891280651
Si	19.482984543	14.183681488	2.371148825
Si	19.482984543	14.183681488	8.561518669
Si	19.144708633	19.473356247	2.437865496
Si	19.144708633	19.473356247	8.628235817
Si	21.425617218	22.134887695	2.313559771
Si	21.425617218	22.134887695	8.503929138
Si	26.044097900	24.694648743	2.312519789
Si	26.044097900	24.694648743	8.502889633
Si	17.977500916	21.504230499	2.182856321
Si	17.977500916	21.504230499	8.373226166
Si	13.608059883	24.501747131	2.250808239
Si	13.608059883	24.501747131	8.441178322
Si	19.652181625	11.540126801	3.919551373
Si	19.336135864	16.825511932	3.915735006
Si	23.741312027	23.409229279	3.860736609
Si	28.331363678	26.004650116	3.861312628
Si	15.799848557	23.023534775	3.801374197
Si	11.393211365	25.940557480	3.796100140
Si	19.482984543	14.183681488	5.466338634
Si	19.144708633	19.473356247	5.533055305
Si	21.425617218	22.134887695	5.408740520
Si	26.044097900	24.694648743	5.407709122
Si	17.977500916	21.504230499	5.278036594
Si	13.608059883	24.501747131	5.345988274
C	19.435127258	15.019349098	0.823478818
C	19.435127258	15.019349098	7.013849735
C	19.798753738	20.325719833	0.883015931
C	19.798753738	20.325719833	7.073379517
C	20.585672379	21.654466629	0.765684605
C	20.585672379	21.654466629	6.956047058
C	25.296428680	24.270614624	0.764926910
C	25.296428680	24.270614624	6.955295086
C	19.045124054	21.642028809	0.642534971

C	19.045124054	21.642028809	6.832901955
C	14.304948807	24.041429520	0.703306139
C	14.304948807	24.041429520	6.893675804
C	19.593980789	12.371941566	2.371798754
C	19.593980789	12.371941566	8.562169075
C	19.295150757	17.662977219	2.368261099
C	19.295150757	17.662977219	8.558630943
C	22.967308044	22.980463028	2.313104868
C	22.967308044	22.980463028	8.503465652
C	27.604623795	25.582304001	2.313615561
C	16.490932465	22.549312592	2.253640175
C	16.490932465	22.549312592	8.444009781
C	12.090415001	25.493301392	2.248765230
C	12.090415001	25.493301392	8.439135551
C	19.435127258	15.019349098	3.918660164
C	19.798753738	20.325719833	3.978199005
C	20.585672379	21.654466629	3.860866785
C	25.296428680	24.270614624	3.860114574
C	19.045124054	21.642028809	3.737721682
C	14.304948807	24.041429520	3.798486233
C	19.593980789	12.371941566	5.466988564
C	19.295150757	17.662977219	5.463450432
C	22.967308044	22.980463028	5.408284664
C	27.604623795	25.582304001	5.408804893
C	16.490932465	22.549312592	5.348820210
C	12.090376854	25.493301392	5.343955040

Table S2. Structure file of tri-SiC-BP (atom, corresponding x, y and z Cartesian coordinates in Å.

H	19.789909363	9.904817581	0.759623945
H	19.789278030	9.904084206	6.950113297
H	29.501964569	26.794349670	0.775626659
H	29.501964569	26.794349670	6.965982437
H	9.923345566	26.799301147	0.765043914
H	9.923345566	26.799301147	6.955406189
H	19.789356232	9.904156685	3.854645252
H	29.501964569	26.794349670	3.870811701
H	9.923345566	26.799264908	3.860226154
P	19.316513062	11.251726151	0.757763982
P	19.319355011	11.252093315	6.948107719
P	19.770877838	16.774515152	0.757234752
P	19.771076202	16.774553299	6.947587967
P	19.882463455	13.974341393	2.302380085
P	19.882581711	13.974341393	8.492777824

P	19.039754868	19.484327316	2.293623686
P	19.039951324	19.484291077	8.483993530
P	19.319000244	11.252056122	3.852983236
P	19.770837784	16.774515152	3.852407694
P	19.882543564	13.974452019	5.397578716
P	19.039674759	19.484291077	5.388822556
B	19.829158783	14.924915314	0.754683971
B	19.829553604	14.924878120	6.945071697
B	19.484010696	20.470523834	0.747256517
B	19.484010696	20.470523834	6.937633514
B	19.725271225	12.129071236	2.304822206
B	19.725467682	12.129071236	8.495702744
B	19.598955154	17.713935852	2.304887056
B	19.599151611	17.713935852	8.495228767
B	19.829433441	14.924878120	3.849826336
B	19.483972549	20.470487595	3.842462778
B	19.726652145	12.129034042	5.400206566
B	19.598995209	17.713899612	5.400067806
C	20.536354065	21.779386520	0.768182456
C	20.536394119	21.779424667	6.958461285
C	25.367544174	24.004190445	0.771036804
C	25.367544174	24.004190445	6.961413860
C	19.023012161	22.083343506	0.771970868
C	19.023012161	22.083343506	6.962286949
C	14.099266052	24.073125839	0.768781364
C	14.099266052	24.073125839	6.959148407
C	23.086280823	22.644369125	2.317190409
C	23.086200714	22.644479752	8.507551193
C	27.581563950	25.471984863	2.321053267
C	27.581563950	25.471984863	8.511423111
C	16.498277664	22.956726074	2.317274094
C	16.498395920	22.956981659	8.507643700
C	11.841653824	25.469636917	2.314869165
C	11.841653824	25.469636917	8.505239487
C	20.536394119	21.779424667	3.863346100
C	25.367584229	24.004154205	3.866224527
C	19.023012161	22.083307266	3.867143869
C	14.099225998	24.073091507	3.863968134
C	23.086280823	22.644332886	5.412370682
C	27.581563950	25.471984863	5.416243076
C	16.498237610	22.956615448	5.412454128
C	11.841653824	25.469636917	5.410058498
Si	23.860006332	23.068918228	0.769737720
Si	23.860006332	23.068918228	6.960123539

Si	28.277582169	25.945215225	0.773645103
Si	28.277582169	25.945215225	6.964014053
Si	15.694698334	23.303972244	0.769579887
Si	15.694658279	23.303936005	6.959956169
Si	11.142001152	25.939748764	0.767142415
Si	11.142001152	25.939748764	6.957514286
Si	21.427907944	22.065732956	2.316549778
Si	21.427747726	22.066062927	8.506900787
Si	26.087808609	24.479661942	2.318843365
Si	26.087808609	24.479698181	8.509222031
Si	18.160875320	22.400873184	2.320217609
Si	18.161111832	22.401496887	8.510578156
Si	13.352585793	24.504608154	2.316224813
Si	13.352585793	24.504644394	8.506594658
Si	23.860046387	23.068880081	3.864924431
Si	28.277542114	25.945215225	3.868833780
Si	15.694619179	23.303789139	3.864766836
Si	11.142001152	25.939714432	3.862324476
Si	21.427946091	22.065660477	5.411711216
Si	26.087808609	24.479661942	5.414032936
Si	18.160755157	22.400653839	5.415388584
Si	13.352585793	24.504571915	5.411414146

Table S3. Structure file of tri-SiC-PbS (atom, corresponding x, y and z Cartesian coordinates in Å.

C	17.567649841	16.048925400	0.558335721
C	22.107393265	18.391424179	0.534626126
C	15.952651024	15.990599632	0.634266019
C	11.373600006	18.391925812	0.637173891
C	19.819610596	17.074075699	2.036492825
C	24.439910889	19.740499496	2.031075001
C	13.661049843	17.074924469	2.136033058
C	9.041753769	19.740400314	2.133827925
C	17.560485840	15.946300507	3.565088987
C	22.118074417	18.398849487	3.557528973
C	15.922317505	15.976025581	3.650094032
C	11.364793777	18.398450851	3.660228014
C	19.818908691	17.070800781	5.091525078
C	24.442523956	19.741926193	5.091543198
C	13.665403366	17.073749542	5.193927288
C	9.040916443	19.741001129	5.194413185
C	17.581478119	15.975549698	6.626439095
C	22.116098404	18.396749496	6.613263130
C	15.906614304	15.972250938	6.727283955

C	11.367340088	18.395750046	6.716196060
C	19.819343567	17.083999634	8.111564636
C	24.426887512	19.732849121	8.115884781
C	13.660916328	17.084449768	8.215884209
C	9.055046082	19.732975006	8.218665123
Si	20.579214096	17.513200760	0.534201264
Si	25.207752228	20.183725357	0.530072987
Si	12.901078224	17.514024734	0.637249470
Si	8.274448395	20.183450699	0.633064508
Si	18.346138000	16.220325470	2.053232908
Si	22.878850937	18.838926315	2.032560110
Si	15.136965752	16.223125458	2.127419949
Si	10.602980614	18.839025497	2.135006905
Si	20.569236755	17.506050110	3.558735132
Si	25.185787201	20.171224594	3.557295084
Si	12.911826134	17.506525040	3.659166098
Si	8.295910835	20.171298981	3.660524845
Si	18.320960999	16.221549988	5.093604088
Si	22.872457504	18.835124969	5.091606140
Si	15.158662796	16.224674225	5.182146072
Si	10.608203888	18.835948944	5.193828106
Si	20.574893951	17.509874344	6.611850262
Si	25.189067841	20.172950745	6.615944862
Si	12.906368256	17.510774612	6.714900017
Si	8.292394638	20.173250198	6.718247890
Si	18.375000000	16.218700409	8.111483574
Si	22.882232666	18.841323853	8.115452766
Si	15.106296539	16.222000122	8.216739655
Si	10.599398613	18.841199875	8.218862534
H	26.494058609	20.926275253	0.458488792
H	6.987940311	20.926399231	0.561334491
H	26.481872559	20.919124603	3.550139904
H	7.000027180	20.919223785	3.652992010
H	26.482675552	20.919775009	6.647030830
H	6.998888493	20.919925690	6.749855995
S	16.915088654	14.709700584	0.314511299
S	16.707567215	14.656350136	3.520871878
S	16.764051437	14.699975014	6.737885952
S	16.675125122	5.696450233	1.858851075
S	16.673717499	5.794724941	5.107662201
S	16.733884811	5.940424919	8.888372421
S	16.963571548	8.747924805	0.429791391
S	16.695013046	8.806349754	3.507282019
S	16.813772202	8.855750084	6.650073051

S	16.829845428	11.750075340	1.980207086
S	16.756284714	11.724124908	5.078880310
S	17.045568466	11.630199432	8.131877899
Pb	16.652690887	4.058350086	8.938133240
Pb	16.660827637	4.400449753	3.506588936
Pb	16.666854858	4.489274979	6.716403008
Pb	16.595603943	7.644750118	1.989665985
Pb	16.644588470	7.729899883	5.106275558
Pb	16.387514114	7.717424393	8.100459099
Pb	16.312549591	10.693974495	0.492780596
Pb	16.622323990	10.671975136	3.517091990
Pb	16.439311981	10.679049492	6.632982254
Pb	16.572635651	13.604049683	1.907360911
Pb	16.607757568	13.592250824	5.140593052
Pb	16.247795105	13.493500710	8.234504700

Table S4. Structure file of tri-SiC-PbSe (atom, corresponding x, y and z Cartesian coordinates in Å.

C	17.568187714	16.043775558	0.536181271
C	22.106256485	18.390699387	0.519805789
C	15.946156502	15.988649368	0.616911292
C	11.374938965	18.390951157	0.622544408
C	19.810638428	17.070749283	2.027699947
C	24.438339233	19.739500046	2.023668051
C	13.670157433	17.072700500	2.128733873
C	9.043327332	19.739500046	2.126502037
C	17.550708771	15.955850601	3.559113026
C	22.115564346	18.397174835	3.555044889
C	15.937451363	15.981123924	3.647699833
C	11.366970062	18.396949768	3.657906055
C	19.810001373	17.068199158	5.093360901
C	24.439342499	19.740074158	5.093639851
C	13.673873901	17.070600510	5.195888996
C	9.043260574	19.739624023	5.196609020
C	17.577093124	15.985274315	6.634674072
C	22.114057541	18.395624161	6.622019768
C	15.910497665	15.990850449	6.741261005
C	11.368711472	18.394824982	6.724791050
C	19.811038971	17.078624725	8.125839233
C	24.427223206	19.732975006	8.130113602
C	13.669487000	17.080024719	8.229834557
C	9.054912567	19.732975006	8.232677460
Si	20.573856354	17.510574341	0.518850923
Si	25.206546783	20.182849884	0.517088711

Si	12.906736374	17.511400223	0.621984601
Si	8.275420189	20.182723999	0.619971275
Si	18.337234497	16.208250046	2.040651083
Si	22.878047943	18.838499069	2.025216103
Si	15.143394470	16.211200714	2.122452021
Si	10.603784561	18.838575363	2.127537012
Si	20.565822601	17.504974365	3.556332111
Si	25.189002991	20.172874451	3.555791855
Si	12.915374756	17.505350113	3.657060146
Si	8.292796135	20.172899246	3.658617020
Si	18.315670013	16.205150604	5.094305992
Si	22.874130249	18.836149216	5.093595028
Si	15.164186478	16.208299637	5.185521126
Si	10.607132912	18.836624146	5.196023941
Si	20.570308685	17.508251190	6.621219158
Si	25.191413879	20.174200058	6.622577667
Si	12.911256790	17.509151459	6.724602222
Si	8.290754318	20.174049377	6.725384712
Si	18.367969513	16.207473755	8.120052338
Si	22.882099152	18.841199875	8.129394531
Si	15.112055779	16.209850311	8.223525047
Si	10.599398613	18.841175079	8.232893944
H	26.491884232	20.925125122	0.457248598
H	6.990216732	20.925125122	0.560077190
H	26.482877731	20.919851303	3.550103903
H	6.999089718	20.919851303	3.652983189
H	26.483377457	20.920175552	6.646950245
H	6.998553753	20.920175552	6.749783993
Se	16.877021790	14.683898926	0.358595997
Se	16.691864014	14.630701065	3.516281843
Se	16.734085083	14.677600861	6.716591835
Se	16.672378540	5.678925037	1.854009032
Se	16.672647476	5.789025307	5.116724968
Se	16.713930130	5.957674980	8.778536797
Se	16.877990723	8.737874985	0.503257513
Se	16.688516617	8.802575111	3.506372929
Se	16.793415070	8.853300095	6.612489223
Se	16.821172714	11.750124931	2.016224861
Se	16.740381241	11.727525711	5.081274033
Se	17.011617661	11.557800293	8.088542938
Pb	16.652791977	4.134250164	8.960393906
Pb	16.664409637	4.445125103	3.513312101
Pb	16.667022705	4.544175148	6.763122082
Pb	16.614555359	7.611800194	2.011887074

Pb	16.644756317	7.713124752	5.092938423
Pb	16.467836380	7.799074650	8.092412949
Pb	16.347871780	10.761349678	0.516969025
Pb	16.618673325	10.663274765	3.526956081
Pb	16.456050873	10.658075333	6.599582672
Pb	16.579500198	13.587975502	1.905578971
Pb	16.627178192	13.587249756	5.134734154
Pb	16.351989746	13.513049126	8.248455048

S2. The computational methods used to calculate the data in Figures 3, 8, 9. (I-V characteristic)

The calculation formula of current *I* is as follows:

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} dE(\mathrm{T(E,V)}(f_1(E) - f_2(E))) \quad (3)$$

The *T*(E,V) is the transmission function representing the probability of electron transmission from source to drain contact through the device, $f_{1,2}(E)$ denotes the Fermi functions of source and drain, while *e* and *h* are the electron charge and Planck constant, respectively.

S3. The computational methods used to calculate the data in Figures 5. (DOS, transmission spectra, LDOS)

In NEGF theory, the transmission function T(E,V) of the system is a sum of transmission probabilities of all channels available at energy *E* under external bias voltage *V* [4]:

$T(E,V)=Tr[\Gamma_L(V)G_R(E,V)\Gamma_R(V)G_A(E,V)]$,

where $G^{R,A}$ is the retarded and advanced Green's function, coupling function $\Gamma_{L,R}$ are the imaginary parts of the left and right self-energies, respectively. Self-energy depends on the surface Green's functions of the electrode regions and comes from the nearest-neighbor interaction between the extended molecule region and the electrodes. There are several methods discussed in literature for the calculation of surface Green's function.[5]

The device density of states (DDOS) $D(E)$ is computed via the spectral density matrix $\rho(E) = \rho^L(E) + \rho^R(E)$ where L/R denotes the contribution from the left/right electrode.

The local density of states (LDOS) is now defined as

$$D(E, \mathbf{r}) = \sum_{ij} \rho_{ij}(E)\phi_i(\mathbf{r})\phi_j(\mathbf{r}),$$

where we note that the basis set orbitals $\phi_i(\mathbf{r})$ are real functions in ATK through the use of solid harmonics.

The device density of states is then obtained by integrating the LDOS over all space:

$$D(E) = \int d\mathbf{r} D(E, \mathbf{r}) = \sum_{ij} \rho_{ij}(E) S_{ij},$$

where $S_{ij} = \int \phi_i(\mathbf{r})\phi_j(\mathbf{r}) d\mathbf{r}$ is the overlap matrix.

Introducing $M_i(E) = \sum_j \rho_{ij}(E) S_{ij}$ we may write this as

$$D(E) = \sum_i M_i(E),$$

where thus $M_i(E)$ can be seen as the contribution to the DDOS from orbital i. $M_i(E)$ is a spectral mulliken population, with

$$M_i = \int M_i(E) f\left(\frac{E-\mu}{k_B T}\right) dE.$$

$M_i(E)$ can be summed over orbitals of a particular angular momentum, and/or over one or several atoms, to give the projected device density of states (PDDOS), which also can be plotted in VNL.

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