

Supporting Information

Enhanced thermoelectric property of graphene oxide patterned by nanoroad

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The total energies of GONRDs by DFT calculations are listed below:

Type I AC-GONRDs:

road width	total energy (Ry)
2	-1028.3656204299436
3	-996.56975440045278
4	-964.75316145938825
5	-932.92047208699546
6	-901.12335656283517
7	-869.30029564936467
8	-837.48414370641876
9	-805.67196074654021

Type I ZZ-GONRDs:

road width	total energy (Ry)
2	-623.33488914303030
4	-591.49396780575717
6	-559.64576999952737
8	-527.81433012180378
10	-495.98671222777466

Type II AC-GONRDs:

road width	total energy (Ry)
2	-1028.3087316726460
4	-964.66378584068809
6	-901.04721088769247
8	-837.41799398863088
10	-773.80553501807549

Type II ZZ-GONRDs:

road width	total energy (Ry)
2	-623.27991137757999
4	-591.44619300957697
6	-559.61269514063338
8	-527.79257421462023
10	-495.96921930240410

The cell parameters and spatial coordinates of four representative GONRD

models with road width $w = 2$ are shown as follows:

Type I AC-GONRD ($w = 2$):

CELL_PARAMETERS (bohr)

48.247564242	0.000000000	0.000000000
0.000000000	8.295500537	0.000000000
0.000000000	0.000000000	28.345903170

ATOMIC_POSITIONS (angstrom)

C	0.022769803	1.457209848	0.203794220
C	2.603378408	1.457116737	0.089604675
C	5.179350485	1.456933577	-0.067084996
C	7.750567375	1.456650476	-0.232643436
C	10.266523232	1.504331863	-0.248224200
C	12.653735630	1.449641190	0.439825921
C	15.238228759	1.456888080	0.414303608
C	17.815403310	1.457115796	0.377761698
C	20.394469140	1.457223954	0.345022998
C	22.974803448	1.457127004	0.284932173
C	1.298881554	0.737948837	-0.160776205
C	3.873467033	0.737989733	-0.298784293
C	6.448607978	0.738008962	-0.455028187
C	9.032272197	0.745212601	-0.580895980
C	11.428564671	0.690626106	0.076547179
C	13.945822674	0.738169651	0.138186950
C	16.521764688	0.737804663	0.082108450
C	19.100379860	0.737760198	0.049322857
C	21.677024423	0.737923280	0.003254390
C	24.254125382	0.737885759	-0.069681769
C	1.298881554	3.651839273	-0.160776205
C	3.873467033	3.651798378	-0.298784293
C	6.448607978	3.651779148	-0.455028187
C	9.032272197	3.644575508	-0.580895980
C	11.428564671	3.699162004	0.076547179
C	13.945822674	3.651618457	0.138186950
C	16.521764688	3.651983447	0.082108450
C	19.100379860	3.652027912	0.049322857
C	21.677024423	3.651864828	0.003254390
C	24.254125382	3.651902349	-0.069681769
C	0.022769803	2.932578383	0.203794220
C	2.603378408	2.932671494	0.089604675
C	5.179350485	2.932854653	-0.067084996
C	7.750567375	2.933137757	-0.232643436
C	10.266523232	2.885456369	-0.248224200
C	12.653735630	2.940147041	0.439825921

C	15.238228759	2.932900153	0.414303608
C	17.815403310	2.932672436	0.377761698
C	20.394469140	2.932564277	0.345022998
C	22.974803448	2.932661227	0.284932173
O	0.067163684	2.194894116	1.458958694
O	2.674061051	2.194894116	1.343768112
O	5.264536117	2.194894116	1.186725360
O	7.864417740	2.194894116	1.025512775
O	12.570595479	2.194894116	1.705570013
O	15.240645499	2.194894116	1.671507150
O	17.826319179	2.194894116	1.633549848
O	20.417247551	2.194894116	1.601169412
O	23.010993710	2.194894116	1.540707289
O	1.241284141	4.389788293	-1.414575649
O	3.803258168	4.389788293	-1.552429934
O	6.399046007	4.389788293	-1.711860827
O	9.079897785	4.389788293	-1.848288334
O	13.880428275	4.389788293	-1.123523238
O	16.490796151	4.389788293	-1.174013412
O	19.080549436	4.389788293	-1.206293028
O	21.647585530	4.389788293	-1.252080862
O	24.211048996	4.389788293	-1.324529655

Type I ZZ-GONRD ($w = 2$):

CELL_PARAMETERS (bohr)

4.858138475	0.000000000	0.000000000
0.000000000	49.577575606	0.000000000
0.000000000	0.000000000	28.345903160

ATOMIC_POSITIONS (angstrom)

C	0.000000000	1.485449467	0.204947612
C	0.000000000	5.921904158	0.374913359
C	0.000000000	10.260500770	-0.494563233
C	0.000000000	14.469530056	0.250881360
C	0.000000000	18.895095009	0.301455234
C	0.000000000	23.305741335	0.120716081
C	1.285407598	0.770263492	-0.133822977
C	1.285407598	5.192075947	0.070114906
C	1.285407598	9.506271232	-0.556768006
C	1.285407598	13.810715222	-0.185821774
C	1.285407598	18.159223312	0.013732557
C	1.285407598	22.570358003	-0.170586825
C	1.285407598	3.709353337	-0.003405203
C	1.285407598	8.060611121	-0.179370195

C	1.285407598	12.361451548	-0.538937955
C	1.285407598	16.678361720	0.058086128
C	1.285407598	21.088180141	-0.099210118
C	1.285407598	25.522121171	-0.176338649
C	0.000000000	2.967635132	0.272365015
C	0.000000000	7.404148432	0.262975848
C	0.000000000	11.607421721	-0.478976424
C	0.000000000	15.948619653	0.359452511
C	0.000000000	20.376487854	0.243959360
C	0.000000000	24.789820367	0.123100884
O	0.000000000	2.170060139	1.490269943
O	0.000000000	6.759661375	1.564120179
O	0.000000000	15.114113742	1.551802980
O	0.000000000	19.684096467	1.524172845
O	0.000000000	24.045921328	1.374492781
O	1.285407598	4.506043712	-1.219224559
O	1.285407598	8.433753517	-1.577245023
O	1.285407598	13.420576600	-1.577767501
O	1.285407598	17.385776687	-1.218766518
O	1.285407598	21.769088585	-1.384602896
O	1.285407598	26.298458314	-1.406587670

Type II AC-GONRD ($w = 2$):

CELL_PARAMETERS (bohr)

49.184672331	0.000000000	0.000000000
0.000000000	8.191480055	0.000000000
0.000000000	0.000000000	28.345903160

ATOMIC_POSITIONS (angstrom)

C	0.020766791	1.446700477	0.181521476
C	2.643064547	1.446479148	0.180533125
C	5.269143036	1.446669876	0.183557324
C	7.889822771	1.446384604	0.195338324
C	10.456721193	1.478920713	-0.014503413
C	12.937339526	1.436237848	0.160144309
C	15.557953023	1.448105343	0.192638566
C	18.182407301	1.446464744	0.180948223
C	20.805393005	1.446804200	0.181075878
C	23.426512427	1.446666587	0.181291661
C	1.314444232	0.720977491	0.180989460
C	3.938288916	0.721141147	0.180978040
C	6.564533091	0.719516381	0.192141706
C	9.184494991	0.731148406	0.160260064
C	11.665013974	0.688577138	-0.014691305

C	14.232231330	0.721143246	0.195552957
C	16.852762230	0.720768094	0.183367859
C	19.477008868	0.721127272	0.180981415
C	22.098791419	0.720905530	0.181200190
C	24.720178228	0.720724602	0.181394593
C	1.314444232	3.613765376	-0.180989460
C	3.938288916	3.613601719	-0.180978040
C	6.564533091	3.615226485	-0.192141706
C	9.184494991	3.603594460	-0.160260064
C	11.665013974	3.646165728	0.014691305
C	14.232231330	3.613599619	-0.195552957
C	16.852762230	3.613974771	-0.183367859
C	19.477008868	3.613615594	-0.180981415
C	22.098791419	3.613837336	-0.181200190
C	24.720178228	3.614018264	-0.181394593
C	0.020766791	2.888042510	-0.181521476
C	2.643064547	2.888263839	-0.180533125
C	5.269143036	2.888073110	-0.183557324
C	7.889822771	2.888358381	-0.195338324
C	10.456721193	2.855822274	0.014503413
C	12.937339526	2.898505138	-0.160144309
C	15.557953023	2.886637643	-0.192638566
C	18.182407301	2.888278242	-0.180948223
C	20.805393005	2.887938785	-0.181075878
C	23.426512427	2.888076398	-0.181291661
O	0.668612725	1.085298174	1.443297202
O	3.288937382	1.084348842	1.442301261
O	5.907437360	1.079661547	1.449437932
O	8.562073123	1.101060099	1.452970130
O	13.559390905	1.067558048	1.452940559
O	16.216274622	1.090430094	1.449760758
O	18.830299857	1.085355543	1.442598218
O	21.452763566	1.085254262	1.443545385
O	24.072760577	1.084586050	1.443699916
O	0.668612725	3.249444753	-1.443297202
O	3.288937382	3.250394084	-1.442301261
O	5.907437360	3.255081379	-1.449437932
O	8.562073123	3.233682826	-1.452970130
O	13.559390905	3.267184879	-1.452940559
O	16.216274622	3.244312832	-1.449760758
O	18.830299857	3.249387383	-1.442598218
O	21.452763566	3.249488663	-1.443545385
O	24.072760577	3.250156876	-1.443699916

Type II ZZ-GONRD ($w = 2$):

CELL_PARAMETERS (bohr)

4.919606450	0.000000000	0.000000000
0.000000000	49.223406759	0.000000000
0.000000000	0.000000000	28.345903160

ATOMIC_POSITIONS (angstrom)

C	0.010332016	1.460593931	0.217247393
C	0.006199819	5.822893328	0.255671195
C	-0.012285183	10.090812003	-0.183500673
C	0.009549920	14.444085575	0.275162238
C	0.008740250	18.809974956	0.205511923
C	0.010362828	23.159305028	0.159220591
C	1.295445485	0.729059048	0.198287562
C	1.290713968	5.090615127	0.274008377
C	1.308431192	9.444760148	-0.182515365
C	1.293541072	13.711591567	0.252059013
C	1.293666571	18.078124666	0.228464227
C	1.294957598	22.427469397	0.161073562
C	1.292630507	3.646058162	-0.088750747
C	1.299189712	7.970702506	-0.286189322
C	1.288694979	12.297659566	-0.216976886
C	1.294908599	16.623567670	-0.093301356
C	1.293743204	20.980611851	-0.188608077
C	1.295780375	25.338528938	-0.186165801
C	0.008321402	2.914115537	-0.107437538
C	0.009666500	7.237220513	-0.209708066
C	-0.001184031	11.564166146	-0.292173240
C	0.010121849	15.891305229	-0.077942089
C	0.008785567	20.248704135	-0.180530609
C	0.010906187	24.606367710	-0.193319010
O	0.653451975	1.064154334	1.471758270
O	0.648940913	5.494838290	1.529594496
O	0.652038145	14.035482826	1.528358944
O	0.650973399	18.479249633	1.480775554
O	0.652373269	22.792413437	1.424645166
O	0.651407235	3.302214892	-1.362860894
O	0.648362084	7.445675755	-1.504892588
O	0.650790451	12.085362111	-1.511919441
O	0.652282438	16.238931834	-1.350175122
O	0.650608754	20.605099703	-1.448509618
O	0.653596664	24.987071515	-1.453781306