

Line group approach for quantum chemical study of intrinsic helical twist of ultrathin tellurium nanorods

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Table S1. Cell parameters of bulk tellurium P3₁21.

	a , Å	c , Å	E_{gap} , eV
Experiment	4.456 [S1]	5.921 [S1]	0.33 [S2]
PBE0	4.666	5.811	1.499
PBE	4.482	5.958	0.271
PBE-D3	4.322	5.943	0.079

[S1] – C.Adenis, V.Langer, O.Lindqvist // Reinvestigation of the Structure of Tellurium. Acta Cryst. C 45 (1989) 941. <https://doi.org/10.1107/S0108270188014453>

[S2] - V.B.Anzin, M.I.Eremets, Yu.V.Kosichkin, A.I.Nadezhdinskii, A.M.Shirokov // Measurement of the energy gap in tellurium under pressure. Phys. Stat. Solidi A 42 (1977) 385. <https://doi.org/10.1002/pssa.2210420143>

Cell parameters of hypothetical bulk tellurium P4₁22 (PBE):

$$a = 4.458 \text{ \AA}$$

$$c = 7.376 \text{ \AA}$$

$$E_{\text{gap}} = 0.048 \text{ eV}$$

$$E_{\text{form}} = 12.5824 \text{ kJ/mol (Formation energy per Te atom, from P3}_{121} \text{ phase)}$$

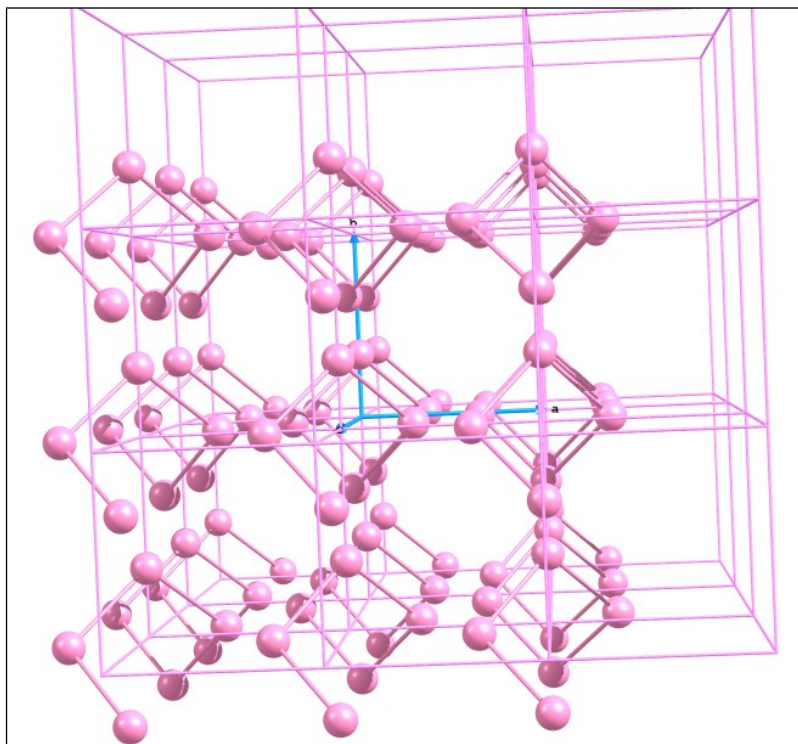


Figure S1. Top view of hypothetical bulk tellurium P4₁22

Interpolation polynomials:

Figure 3:

$$S(\text{hex}) = 0.14053 + 0.17854 * N(\text{hex})$$

$$S(\text{trig}) = -0.09616 + 0.16161 * N(\text{trig})$$

Figure 4:

$$E_f(\text{hex}) = 33.16571 * (1 + N(\text{hex}))^{-0.59599}$$

$$E_f(\text{trig}) = 32.11394 * (1 + N(\text{trig}))^{-0.58732}$$

Figure 5:

$$\text{Te1: } E_{\text{form}}(\varphi) = 132.1242 - 2.1060 * \varphi + 0.0099 * \varphi^2$$

$$\text{Te3: } E_{\text{form}}(\varphi) = 395.9012 - 6.5599 * \varphi + 0.0281 * \varphi^2$$

$$\text{Te6: } E_{\text{form}}(\varphi) = 1575.5734 - 26.2547 * \varphi + 0.1100 * \varphi^2$$

$$\text{Te7: } E_{\text{form}}(\varphi) = 2254.7654 - 37.6360 * \varphi + 0.1577 * \varphi^2$$

$$\text{Te10: } E_{\text{form}}(\varphi) = 3188.3318 - 53.1892 * \varphi + 0.2224 * \varphi^2$$

$$\text{Te19: } E_{\text{form}}(\varphi) = 8363.9214 - 139.5169 * \varphi + 0.5822 * \varphi^2$$

Parameters of the energy minima of nanorods obtained in crystallographic paradigm

Te1 (L3₁21):

$$E_{\text{form}} = 22.05375 \text{ kJ/mol}$$

$$E_{\text{gap}} = 1.5431 \text{ eV}$$

$$T = 5.72734959 \text{ \AA}$$

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	0.000000000000	0.5773575772259	-1.000012657890
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Te7hex (L3₁21):

$$E_{\text{form}} = 9.17727 \text{ kJ/mol}$$

$$E_{\text{gap}} = 0.6671 \text{ eV}$$

$$T = 5.82654916 \text{ \AA}$$

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.0063272617660	5.12983001028200	-0.976466543419100
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Te	0.0000000000000	2.84689771027900	-4.93097147815400
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Te	1.93558361943699	2.89701169868200	-2.89245925432900
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Te	-1.94218305333314	3.23600734007700	0.0000000000000
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Te	0.0000000000000	0.637133639806200	-1.10354783535600
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Te19hex (L3₁21):

$$E_{\text{form}} = 5.55131 \text{ kJ/mol}$$

$$E_{\text{gap}} = 0.5803 \text{ eV}$$

$$T = 5.86943863 \text{ \AA}$$

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.00682253200120	9.61102475766800	-0.9688334270407
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Te	-0.04722101695221	7.41649564806900	-4.8877178419260
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Te	0.0000000000000	5.09374139753200	-8.8226189011420
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Te	1.92925919426999	7.41186545006300	-2.8698006566270
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Te	1.94603596966695	5.15300018145200	-6.7886132381380
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Te	-1.95647954333314	7.69507425739200	0.0000000000000
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Te	-1.96692900526183	5.53722147760700	-3.9184130281550
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Te	-0.00470407414486	5.14980295353200	-1.0845595656400
Te	0.00000000000000	2.92843375601900	-5.0721960520240
Te	1.94379045137579	2.90140593443900	-2.8873086431080
Te	-1.95647954333314	3.26934930910400	0.00000000000000
Te	0.00000000000000	0.626942549658200	-1.0858963494350

Te37hex (L3₁21):

Eform = 3.94249 kJ/mol

Egap = 0.5038 eV

T = 5.89346233 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.00424413389242	14.0743469402400	-0.966865170537200
Te	-0.04888329838237	11.8934427702300	-4.87963655315600
Te	-0.04762946131554	9.66318522245500	-8.77211159547100
Te	0.00000000000000	7.33035057720700	-12.6965396370100
Te	1.93786192358090	11.8850905259500	-2.86630109628700
Te	1.92454323191078	9.68014847179200	-6.73753697887100
Te	1.95205175728101	7.39290866411100	-10.6661929945500
Te	-1.96448744333314	12.1547933838800	0.00000000000000
Te	-1.98010286549180	10.0007095952700	-3.91474285303200
Te	-1.98165350882034	7.80509128460100	-7.79750588976100
Te	-0.00289570768185	9.63036638976600	-1.07922072502700
Te	0.014847793424675	7.39477190257900	-5.01580407529600
Te	0.00000000000000	5.18239321451400	-8.97616835233800
Te	1.98809734551526	7.37938328453900	-2.86052095373300
Te	1.94798725494296	5.15732697655100	-6.79614364134700
Te	-1.96448744333314	7.74450113603300	0.00000000000000
Te	-1.93083910754023	5.51131738228600	-3.93320786039700
Te	-0.00269701551945	5.13739492561100	-1.08594704766200
Te	0.00000000000000	2.89711021250500	-5.01794208318500
Te	1.96334381340128	2.88749761057900	-2.84257531032000
Te	-1.96448744333314	3.25966864968600	0.00000000000000
Te	0.00000000000000	0.627355873875100	-1.08661224797800

Te61hex (L3₁21):

Eform = 3.04908 kJ/mol

Egap = 0.4457 eV

T = 5.90790299 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.00269961801821	18.5408777239200	-0.965606674713100
Te	-0.04441918082841	16.3621018273300	-4.88213293615000
Te	-0.05311696084003	14.1437767435200	-8.76437128858700
Te	-0.04360528297932	11.9054586224800	-12.6467638821200
Te	0.00000000000000	9.56481069848800	-16.5667380945600
Te	1.94427174703246	16.3559796363500	-2.87021103592600
Te	1.92816322662634	14.1591178946100	-6.72872819846500
Te	1.92859641106529	11.9312267799500	-10.6078406477200
Te	1.95638554139935	9.62907243658400	-14.5400742818800
Te	-1.96930099666647	16.6230576033400	0.00000000000000
Te	-1.98490421647116	14.4693288912800	-3.91670136558500
Te	-1.99499008520504	12.2751755307500	-7.79006225202200
Te	-1.98483809676404	10.0570233559000	-11.6724236569600

Te	-0.00181137379408	14.1044424984900	-1.07595975075700
Te	0.021756642911057	11.8689027059700	-4.99921241525900
Te	0.014486057045516	9.64912504105600	-8.90610457672300
Te	0.00000000000000	7.42304305548800	-12.8570877188800
Te	1.99971051057818	11.8597045606300	-2.85315090031900
Te	1.98971588316074	9.63402707662900	-6.75126858273900
Te	1.95360140371690	7.40181224774300	-10.6811455055200
Te	-1.96930099666647	12.2159457639100	0.00000000000000
Te	-1.92834756099215	9.98176897819400	-3.92148510146900
Te	-1.93421127145284	7.76945942546900	-7.82860046655700
Te	-0.00396231924073	9.62086432657500	-1.08113263263300
Te	-0.00116627137816	7.38419257314800	-5.00741336461300
Te	0.00000000000000	5.15338019789900	-8.92591633348100
Te	1.97222044160898	7.37615229481800	-2.83750101904300
Te	1.96452768058208	5.13905597299500	-6.75262647008900
Te	-1.96930099666647	7.74226037289300	0.00000000000000
Te	-1.96604824296149	5.50397584178700	-3.91677216840200
Te	-0.00073753141304	5.13601848586700	-1.08742470034300
Te	0.00000000000000	2.89036069346200	-5.00625157327700
Te	1.96858630281471	2.88299807890900	-2.83056074399000
Te	-1.96930099666647	3.25882472276800	0.00000000000000
Te	0.00000000000000	0.626418108644800	-1.08498799095400

Te91hex (L3₁21):

E_{form} = 2.48365 kJ/mol

E_{gap} = 0.4132 eV

T = 5.91755254 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

252	-0.00151026816367	23.0054471033500	-0.96517185667330
252	-0.04070702855894	20.8325595572400	-4.88273604704200
252	-0.05118770911336	18.6139160463100	-8.76718275076700
252	-0.05042364520461	16.3899126433400	-12.6379091303000
252	-0.04147472883461	14.1428579556500	-16.5182561852200
252	0.00000000000000	11.7988549687100	-20.4362162769400
252	1.94832477180439	20.8262259234000	-2.87234348609700
252	1.93180437148476	18.6320572735900	-6.73138833957400
252	1.92913034288644	16.4131277437800	-10.5950339134100
252	1.93235132182993	14.1732657396900	-14.4793959761100
252	1.95945679767738	11.8641232829700	-18.4121421353600
252	-1.97251751333314	21.0895400109500	0.00000000000000
252	-1.98700374962774	18.9412856189200	-3.91948987814300
252	-2.00001940537963	16.7453997723000	-7.79177719215800
252	-1.99819374215594	14.5313694254400	-11.6634508697700
252	-1.98728797185922	12.2994220944000	-15.5448831819200
252	-0.00099871356759	18.5745430471200	-1.07392993470400
252	0.024156661934982	16.3418708717500	-4.99427448998300
252	0.019437373489255	14.1204415549300	-8.88334331027800
252	0.015807589390894	11.8945470464100	-12.7843143816600
252	0.00000000000000	9.66034595409800	-16.7322100111900
252	2.00469250408132	16.3354020007500	-2.85346119264900
252	1.99988737734647	14.1120211993600	-6.73634643624000
252	1.99226626424354	11.8823641483800	-10.6292479757600

252	1.95766103903446	9.64140233241600	-14.5591589023000
252	-1.97251751333314	16.6843402130100	0.0000000000000
252	-1.92873329367260	14.4531940414400	-3.91891619775000
252	-1.93200213163591	12.2379879269600	-7.80991181942700
252	-1.93795560552173	10.0184458438200	-11.7090210508900
252	-0.00384880087519	14.0987726709600	-1.07833543886900
252	0.003143606326083	11.8595348612500	-4.99023539098500
252	0.002015337250171	9.62977473227200	-8.90846191207000
252	0.00000000000000	7.39911844230400	-12.8156490732900
252	1.98271883161811	11.8570784037500	-2.82860796133100
252	1.97662812920366	9.61654921528000	-6.74081786686200
252	1.96619209531343	7.38504488903900	-10.6440584516100
252	-1.97251751333314	12.2166239770700	0.0000000000000
252	-1.96478304605072	9.98020669327800	-3.90611561766500
252	-1.96295904314433	7.75034123170700	-7.81702254452900
252	-0.00194503836760	9.62332339369500	-1.08489010444200
252	0.002496152319081	7.38234382976300	-5.00154062279800
252	0.00000000000000	5.14443620527900	-8.91042488384000
252	1.97637441783520	7.37538859050100	-2.82853624916900
252	1.97048122289241	5.13322862497000	-6.73452877724400
252	-1.97251751333314	7.74526675552800	0.0000000000000
252	-1.96672608165019	5.50295347033700	-3.90933077634700
252	-0.00066121420584	5.12898010292500	-1.08561091695600
252	0.00000000000000	2.88346996926900	-4.99431648887300
252	1.97178157859504	2.87872666785200	-2.82216814056900
252	-1.97251751333314	3.25178242176500	0.0000000000000
252	0.00000000000000	0.626438380059400	-1.08502310207400

Te3trig (L₃₁):

Eform = 13.26267 kJ/mol

Egap = 1.2398 eV

T = 5.7605033 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	0.00386488124104	2.85214451065900	0.265905075627100
Te	-0.0096365800538	0.554932119895000	-3.57785582951800
Te	1.92593946547929	0.652324141537900	-1.51192281007700

Te6trig (L₃₁):

Eform = 9.64911 kJ/mol

Egap = 1.0892 eV

T = 5.78653469 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.0409961320452	5.08179239100000	1.52161928781000
Te	0.03366468128155	2.90578524446000	-2.32295705186900
Te	-0.0596971613364	0.52535064822830	-6.11410236473800
Te	1.98046519682890	2.94528339884600	-0.223805921405800
Te	1.88866422367171	0.64236160943750	-4.05116601816200
Te	-1.8732559117340	1.04849989361400	-1.28727160830400

Te10trig (L₃₁):

Eform = 7.63565 kJ/mol

Egap = 0.8747 eV

T = 5.81839619 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.06850280097890	7.28735360740000	2.79247969395100
Te	0.011812479211701	5.16704453104100	-1.06467369994600
Te	-0.00298718115445	2.89065355777400	-4.87697614243100
Te	-0.09148827914013	0.519529483415700	-8.65283920473500
Te	1.95050772558200	5.18398541215500	1.02968746199200
Te	1.96765331100453	2.96450170296200	-2.78816070968400
Te	1.87011604464490	0.627798553215500	-6.59247991039800
Te	-1.91169999033041	3.29584403392100	-0.03174423532586
Te	-1.91499679534981	1.04650626485600	-3.85710363010300
Te	0.129050883177246	0.619959768503500	-1.08750637595900

Te15trig (L3₁):

Eform = 6.35218 kJ/mol

Egap = 0.8333 eV

T = 5.83970204 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.0962539527226	9.50299432165600	4.07197535693700
Te	-0.0071291403576	7.38894491016200	0.204614772967400
Te	-0.0030472558511	5.18398329366200	-3.62746720349300
Te	-0.0290739564713	2.87893351709900	-7.42778293391500
Te	-0.1195661319228	0.514600753020300	-11.2045245691500
Te	1.93577892684803	7.40204634795100	2.29707351464100
Te	1.94714046993869	5.23137042653200	-1.53345933531200
Te	1.95896833335152	2.95996415438200	-5.34349550230500
Te	1.84862967679173	0.619414653312000	-9.14907897543500
Te	-1.9407604229744	5.51593582011100	1.23401370471200
Te	-1.9328916124748	3.32789920761500	-2.61212927032700
Te	-1.9448766263719	1.04007686615600	-6.41696011705600
Te	0.11065873305984	2.87805011261800	0.205876521165200
Te	0.09798270818009	0.608804924172200	-3.67613619800300
Te	2.06757494431009	0.633202660322000	-1.51678483521600

Te21trig (L3₁):

Eform = 5.43489 kJ/mol

Egap = 0.7646 eV

T = 5.8563184 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.113737047119240	11.7147158900700	5.35338735636300
Te	-0.0298045864429719	9.61168197049100	1.48784170309500
Te	-0.00797013760987467	7.42403537100200	-2.36324182146600
Te	-0.0168427134864	5.17994008757700	-6.18514100509100
Te	-0.0539656388493	2.86715558953900	-9.98351307810500
Te	-0.1401710947398	0.515910700106100	-13.7611125666500
Te	1.91667804085544	9.61944159698000	3.57502274367000
Te	1.94082628060338	7.46420125122600	-0.266970085203200
Te	1.95025253920375	5.24041599393900	-4.09416595770000
Te	1.93984789931380	2.94693969616500	-7.90555016415400
Te	1.83322889836176	0.616985435998200	-11.7078970404700
Te	-1.96867962135147	7.73905401567800	2.50855632410000
Te	-1.94965011226890	5.56610944550800	-1.35102044934700

Te	-1.95031762342815	3.33072606588400	-5.17788943551400
Te	-1.97562590800415	1.03023596401300	-8.97805944313500
Te	0.09221641660952	5.10828707895700	1.48111286732200
Te	0.09440790690431	2.89237396454100	-2.39458641509400
Te	0.07696613642783	0.59892207281170	-6.23771819455400
Te	2.04767079040982	2.90930216329600	-0.234280083598200
Te	2.05974539617843	0.62822838396050	-4.07900677148300
Te	-1.84086355490463	1.02098287699500	-1.30489561710800

Te28trig (L3₁):

Eform = 4.75517 kJ/mol

Egap = 0.6933 eV

T = 5.86903378 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.1304551248016	13.9339694720300	6.64065832207300
Te	-0.0453534815322	11.8285783317400	2.77201398341700
Te	-0.0227506550656	9.65943350167600	-1.08171695809300
Te	-0.0095522305601	7.43365026906100	-4.92787348517700
Te	-0.0367239539569	5.16840453373400	-8.74597024391600
Te	1.79874365687455	13.8757958605100	8.61081087217400
Te	1.90384849108099	11.8385944304000	4.85646850722900
Te	1.92629892451947	9.69078313942600	1.01181920293300
Te	1.95403122834591	7.48903090829600	-2.83223837225800
Te	1.93675117340991	5.23376347512300	-6.66239973762000
Te	-2.09316262280907	12.0515484380700	7.66945914674900
Te	-1.99046053425974	9.95975714060400	3.79007965440300
Te	-1.96864967267422	7.80049509751100	-0.07758696843351
Te	-1.95495299383392	5.58470028826500	-3.92260866074900
Te	-1.97469627474031	3.32218763368500	-7.74247545589200
Te	-0.04082089853886	9.48235430760900	6.65848268638500
Te	0.070036277141640	7.33663748908300	2.76005167985900
Te	0.085727454312968	5.13901831011900	-1.12173241651700
Te	0.080735473394157	2.89230355877400	-4.96322983233100
Te	1.88390114059222	9.43321227562800	8.74936378494200
Te	2.01018217308411	7.32685333203800	4.91381980684500
Te	2.03760055175101	5.14637089959800	1.03816708485800
Te	2.04695598368159	2.91974954113000	-2.80184451846500
Te	-1.98690685196293	7.59760728714000	7.77831886109200
Te	-1.86968121351931	5.44624353976200	3.85821537546200
Te	-1.85236109703529	3.26020801466100	-0.03186684897866
Te	-1.85798804902178	1.02238261717200	-3.88042232984300
Te	0.099703126124239	0.618331149185900	-1.08591003962200

Te36trig (L3₁):

Eform = 4.22637 kJ/mol

Egap = 0.6442 eV

T = 5.87914442 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.14319436534905	16.1530642921300	7.92728784954000
Te	-0.06087597165184	14.0507985310500	4.06048245575100
Te	-0.03399904515116	11.8817291226100	0.202695231893700

Te	-0.01544034920190	9.68153573202000	-3.65025134581000
Te	-0.02218637073582	7.42905983489900	-7.49413219101000
Te	-0.05356271006124	5.15862930953300	-11.3093761944900
Te	-0.08814660356572	2.85666326702300	-15.1080497248100
Te	-0.17164640382687	0.522297018684800	-18.8868421276000
Te	1.89104011131222	14.0595477401400	6.14126305295000
Te	1.91630271398382	11.9131819338000	2.29497141844000
Te	1.94574240215127	9.72594046437000	-1.55535764300300
Te	1.94743552498167	7.49196161651800	-5.40555982398000
Te	1.92546294779327	5.22399777488700	-9.22945920307200
Te	1.91194722011191	2.93098710546100	-13.0356548494400
Te	1.80849442489264	0.617381579357300	-16.8382016888400
Te	-2.00921846432257	12.1835401286900	5.07440822445900
Te	-1.98551452494393	10.0254868504600	1.20489379832400
Te	-1.96509385330533	7.83107500638200	-2.65330344997200
Te	-1.97164946992314	5.58379866995300	-6.49207375597900
Te	-1.99339074436945	3.31390955312300	-10.3075959108600
Te	-2.01675542107590	1.02280433206400	-14.1077943439300
Te	0.054110513705976	9.56157852216600	4.04103618722200
Te	0.069121418091976	7.37614197277200	0.156289965566600
Te	0.081507422995507	5.15021935498900	-3.69517960558700
Te	0.061987657238929	2.88826866386400	-7.53175807215900
Te	0.036878581915817	0.587753579368100	-11.3675144445100
Te	2.02084981363876	7.37770338810500	2.31586071671500
Te	2.04507166779145	5.17062491510900	-1.53213511897200
Te	2.03442520477959	2.91787135311300	-5.37231114143400
Te	2.02989505131339	0.612112694073900	-9.21215655806000
Te	-1.87166975231117	5.49660294782900	1.24275211028700
Te	-1.86060895411707	3.27513922038200	-2.61131270249100
Te	-1.88057077966334	1.02001905168100	-6.45272361354600
Te	0.094661665083220	2.86388050422000	0.201569058127100
Te	0.090284378665278	0.612015207447400	-3.66740161268900
Te	2.05744948312835	0.629781445100600	-1.50268806646900

Te45trig (L3₁):

Eform = 3.80537 kJ/mol

Egap = 0.6079 eV

T = 5.88732178 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.15415969883826	18.3751952130400	9.21643897182100
Te	-0.07261008936742	16.2729149636300	5.34947692462500
Te	-0.04746091630919	14.1076895120400	1.49240607873100
Te	-0.02127939228466	11.9122716554700	-2.36806004106000
Te	-0.02122149456855	9.68561048256500	-6.22133105246900
Te	-0.03534027761347	7.42098066559200	-10.0612760011200
Te	-0.06830333512093	5.15072043763200	-13.8751556561700
Te	-0.10058650381731	2.85502287067500	-17.6748153461800
Te	-0.18317245962912	0.526363511997800	-21.4540081140100
Te	1.88137734967503	16.2823063157600	7.42805645772700
Te	1.90483569482624	14.1370407144800	3.58149131817700
Te	1.93936469815752	11.9548164928800	-0.273181938409800
Te	1.94509467087889	9.73838300960400	-4.13243588273500

Te	1.94015244351765	7.48694732129000	-7.97712158746500
Te	1.91291568913275	5.21482605943400	-11.7987278809100
Te	1.90115945511610	2.92750986363100	-15.6042155209000
Te	1.79916222059339	0.619430498075700	-19.4068841212100
Te	-2.02446470300512	14.4078287200000	6.36125521031900
Te	-2.00118279189360	12.2521289043100	2.49080683627200
Te	-1.97623233858968	10.0639417712900	-1.37314165897100
Te	-1.97475969433489	7.83950855381400	-5.22696924764600
Te	-1.98593663672009	5.57771350180800	-9.05993734842300
Te	-2.01114930050401	3.30695809844000	-12.8755057481500
Te	-2.03196040377686	1.02237433281200	-16.6761382367300
Te	0.039164700925343	11.7882567074100	5.32513430858700
Te	0.056196458903969	9.60561428187100	1.43796453258300
Te	0.071681389383220	7.39670371555400	-2.42023116502300
Te	0.068253924683621	5.15244011532800	-6.26742928685000
Te	0.046079832999100	2.88198284515500	-10.0994115481400
Te	0.021623354028576	0.585385866549700	-13.9359632659300
Te	2.00881523426914	9.60444574277600	3.59640078417300
Te	2.03313505583284	7.41018450138800	-0.256299748948500
Te	2.03799308657712	5.17740081166600	-4.10629943486400
Te	2.02316319189435	2.91269009874100	-7.94104870505800
Te	2.01713365962017	0.607422887028700	-11.7822669535900
Te	-1.88816611900098	7.72620241336600	2.52177021703000
Te	-1.87312967093282	5.52083178732000	-1.33980148462800
Te	-1.87801553918284	3.27968576416000	-5.18731063240200
Te	-1.89859282237691	1.01532300072400	-9.02190381376500
Te	0.080039137340889	5.10178283271200	1.48589803214400
Te	0.092727695700313	2.86844786269200	-2.38443951314100
Te	0.073307138126676	0.606410509743300	-6.24353159790300
Te	2.05798723923916	2.88125994828400	-0.219912545755100
Te	2.04746705101357	0.623238156339500	-4.08117487733800
Te	-1.86378440457445	0.991911095275200	-1.29559672186200

Te55trig (L3₁):

Eform = 3.46056 kJ/mol

Egap = 0.5733 eV

T = 5.89399223 Å

Cartesian coordinates of irreducible part. Ox - axis of periodicity.

Te	-0.1631549494236	20.5988116791600	10.5059365612500
Te	-0.0830500164880	18.4977611987500	6.63952376077400
Te	-0.0578917421509	16.3322214259700	2.78228304053100
Te	-0.0313361968851	14.1434513462100	-1.07904874465900
Te	-0.0213526131169	11.9236397453500	-4.94248871584300
Te	-0.0296601980832	9.68254683006400	-8.79251934024000
Te	-0.0482849822361	7.41259081707900	-12.6296790082300
Te	-0.0801897175918	5.14511270317500	-16.4435337338100
Te	-0.1107924490063	2.85444041129800	-20.2440327998300
Te	-0.1928965653948	0.530486674368400	-24.0232920881000
Te	1.87271887534622	18.5070184058200	8.71608735041400
Te	1.89606765296528	16.3619437178100	4.86954260794500
Te	1.93006685697749	14.1822720644900	1.01349689808500

Te	1.94321162072973	11.9741750779400	-2.85234696654300
Te	1.94219570888286	9.73977370364200	-6.70747616056400
Te	1.92975388439045	7.47906242239300	-10.5495622273600
Te	1.90286885706510	5.20765138540600	-14.3690709259400
Te	1.89190681009894	2.92536632958300	-18.1747750435400
Te	1.79138347731601	0.621769299301400	-21.9774259266800
Te	-2.03738854727830	16.6340970576500	7.64924086078100
Te	-2.01433637711123	14.4784287741800	3.77910036002900
Te	-1.98819138623242	12.2950282013900	-0.0880959644193900
Te	-1.98031803514888	10.0796366047400	-3.95010157298400
Te	-1.98410794005687	7.83885988263500	-7.79841436457900
Te	-2.00111818697572	5.57028752134700	-11.6299016966800
Te	-2.02514010525092	3.30211237668800	-15.4451980247400
Te	-2.04479298212169	1.02291750058800	-19.2468555560600
Te	0.02755364700666	14.0154341784800	6.61095790775100
Te	0.04280151876245	11.8350058392500	2.72330615986700
Te	0.06307501283253	9.63225896270600	-1.14018565877700
Te	0.06371380843475	7.40600681064500	-4.99610408665900
Te	0.05586786324450	5.14868416959700	-8.83780359602700
Te	0.03165713409480	2.87685626887400	-12.6695542060400
Te	0.00978788257418	0.584385973978400	-16.5064540615700
Te	1.99699333026912	11.8321608075700	4.88039586308500
Te	2.02392498697331	9.64207265070900	1.02360629940300
Te	2.03048440965475	7.42515621795100	-2.83329234365400
Te	2.03049398770863	5.17712257204800	-6.67781790180700
Te	2.01121538649388	2.90664256325800	-10.5126795445500
Te	2.00708190541848	0.604816655577300	-14.3537974379900
Te	-1.90401756429252	9.95648042155600	3.80454549821700
Te	-1.88515365261669	7.75651267945300	-0.0621311318405000
Te	-1.88502358057293	5.53306131659100	-3.91861623969200
Te	-1.89240557213714	3.27803398659300	-7.75871738664500
Te	-1.91540253551399	1.01122232109800	-11.5937766598900
Te	0.06689344733236	7.33326437503800	2.76836714199300
Te	0.08316736522941	5.11467848436800	-1.10216495784600
Te	0.08026730129917	2.86924498802000	-4.96399180683900
Te	0.05865538912404	0.601199212601200	-8.81527910459100
Te	2.04723472312144	5.12331389708900	1.06241154319100
Te	2.05215384211175	2.88346530587100	-2.80116684681800
Te	2.03698306062062	0.617807766649200	-6.65410409697100
Te	-1.8744341402816	3.23699537241400	-0.0140538287106500
Te	-1.8773419224710	0.992922515751600	-3.87937658073300
Te	0.10159444235498	0.622085503308800	-1.08883101518200

Parameters of the energy minima of nanorods obtained in helical paradigm

Te1 (5th family):

E_{form} = 20.146877773283506 kJ/mol

E_{gap} = 1.431695235614831 eV

Q = 3.419391289636317

f = 1.81700283775590 Å

φ = 105.2818965443084°

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	0.0000000	1.306846524187271	0.0000000
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Te3trig (1st family):

E_{form} = 13.076771873226335 kJ/mol

E_{gap} = 1.231400158005961 eV

Q = 3.062496674754749

f = 1.905387798516305 Å

φ = 117.5511480445377°

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	1.95339656355316	2.59386030436499	-1.13907453084472
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Te	3.94048651888639	3.64092014765182	0.464703329496192
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Te	0.13804788900327	1.46283037652809	0.779776877075610
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Te6trig (1st family):

E_{form} = 9.597500532841423 kJ/mol

E_{gap} = 1.095952306161735 eV

Q = 3.017347287900561

f = 1.926183074811832 Å

φ = 119.3100977947037°

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	1.97820806647724	1.03299546291322	-1.30602197594149
----	------------------	------------------	-------------------

Te	-1.89504152302698	2.92795633496996	-2.31859335739733
----	-------------------	------------------	-------------------

Te	0.055521679371935	2.93847975090796	-0.22628086165826
----	-------------------	------------------	-------------------

Te	1.90054258294822	3.21356856588275	2.56137011992041
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Te	-1.99907882518562	5.03037005354173	1.56205895671508
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Te	-0.04015198058442	5.06479813903860	3.50267598858565
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Te7hex (5th family):

E_{form} = 9.112863311737783 kJ/mol

E_{gap} = 0.687939023328269 eV

Q = 3.014404444147208

f = 1.938568918612174 Å

φ = 119.4265755210715°

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	0.0000000	1.27951281375057	0.0000000
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Te	0.0000000	5.73682995064376	0.0000000
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Te	-0.0182031449204	3.40765873398894	3.9200564911
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Te	-1.9385689108055	1.57920896584789	2.7996073605
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Te	1.94500529016631	3.98161556318303	1.0186471473
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Te10trig (1st family):

Eform = 7.598433380537244 kJ/mol

Egap = 0.906027859872495 eV

Q = 3.009972810227546

f = 1.951518401057611 Å

$\varphi = 119.6024092897985^\circ$

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	0.117600609004519	0.627835539071548	1.08793533841398
Te	-0.08803449625095	7.25434480618725	4.77020158103782
Te	-2.04720533698181	7.23781906796245	2.82925615279183
Te	1.86944012420124	5.41445355066728	3.82305987712677
Te	0.003960271556720	2.79933326200258	4.96789569078841
Te	-1.92079638998588	2.79207632709430	2.87337073281048
Te	1.96851083392623	0.960252310120637	3.96476854926442
Te	-0.01581350850245	-1.63292993999542	4.99184769150893
Te	-1.92701692005139	-1.64104294999902	2.84395655990681
Te	1.93214566310191	-3.45473634625432	3.97962274574521

Te19hex (5th family):

Eform = 5.534058478968291 kJ/mol

Egap = 0.582504603207894 eV

Q = 3.004150868469393

f = 1.955609174294852 Å

$\varphi = 119.8341946732586^\circ$

Cartesian coordinates of irreducible part of monomer. Ox - axis of periodicity.

Te	0.0000000	1.25579755331989	0.0000000
Te	0.0000000	5.87087402026286	0.0000000
Te	0.0000000	10.2205045042560	0.0000000
Te	1.94402810021652	3.95783007738076	1.05405920190190
Te	1.95340024329252	8.48008866963735	1.04063781289705
Te	-0.04661004540523	7.95831002745133	3.95646634586188
Te	-0.00595899904532	3.51319681742652	3.90374294792337
Te	-0.01394149723874	5.63369495306403	7.80706504049454
Te	0.021170716669161	1.20594498763728	7.84729114863418
Te	-1.95561082014132	1.62327837911003	2.83045284431384
Te	-1.95561082014132	3.81526673859926	6.65265442877013
Te	-1.96806703789562	6.16274449950886	2.84465401227543

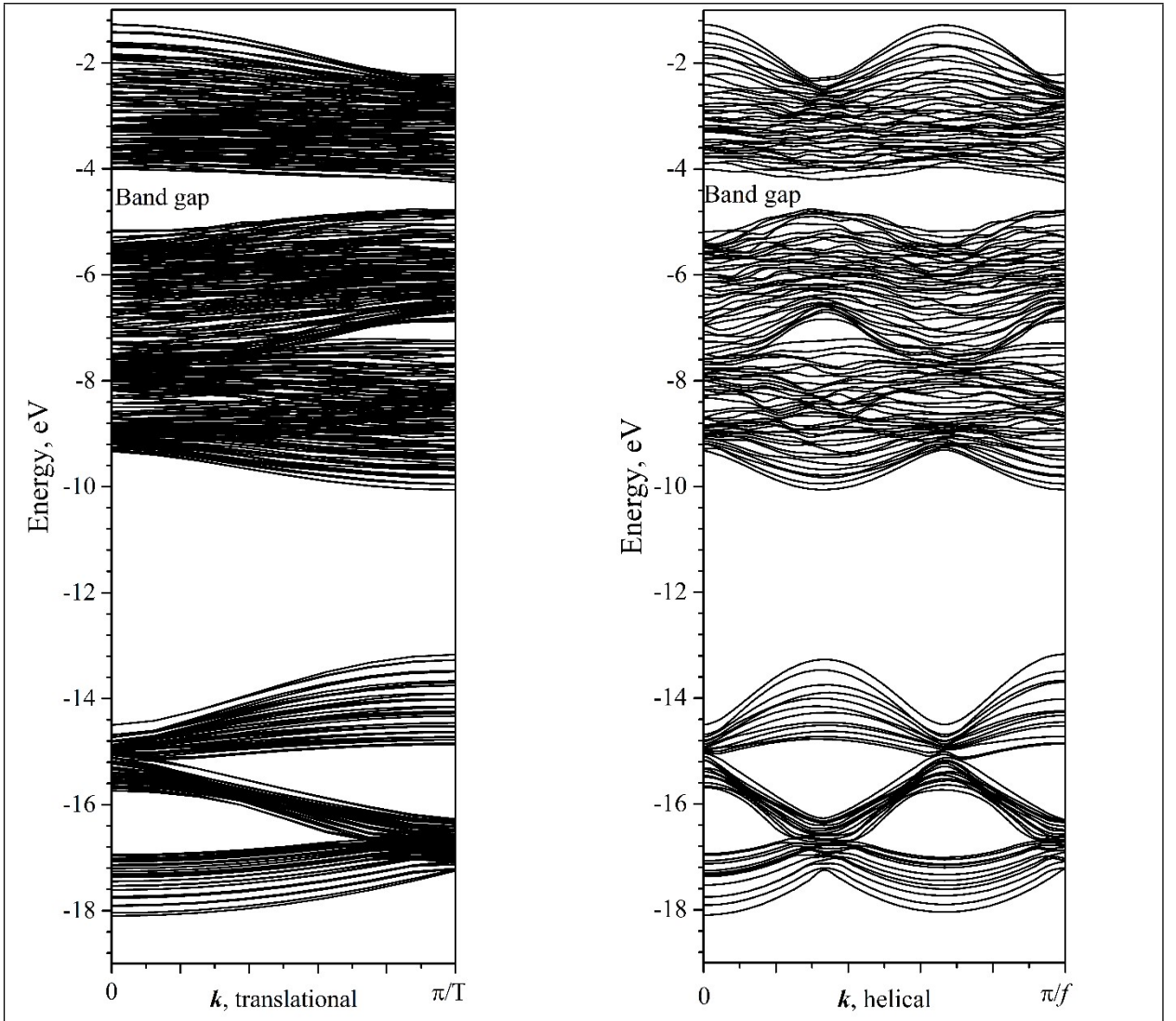


Figure S2. Electronic states of Te₃₇hex, L₃₁₂₁. **Left)** TBZ; **Right)** HBZ.