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Authors	Noor-A-Alam, Mohammad;Olszewski, Oskar Zbigniew;Campanella, Humberto;Nolan, Michael
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Supporting Information

Large Piezoelectric Response and Ferroelectricity in Li and V/Nb/Ta co-doped *w*-AlN

Mohammad Noor-A-Alam[1*], Oskar Z. Olszewski[1] , Humberto Campanella[1] and Michael Nolan[1,2] *

1. Tyndall National Institute, Lee Maltings, Dyke Parade, University College Cork, Cork, T12 R5CP, Ireland

2. NIBEC, School of Engineering, Ulster University, Shore Road, Antrim, Northern Ireland

**Corresponding author: Mohammad Noor-A-Alam (mda.alam@tyndall.ie) and Michael Nolan (michael.nolan@tyndall.ie)*

E-mail: mda.alam@tyndall.ie;michael.nolan@tyndall.ie

The average Z_{33} of each atoms

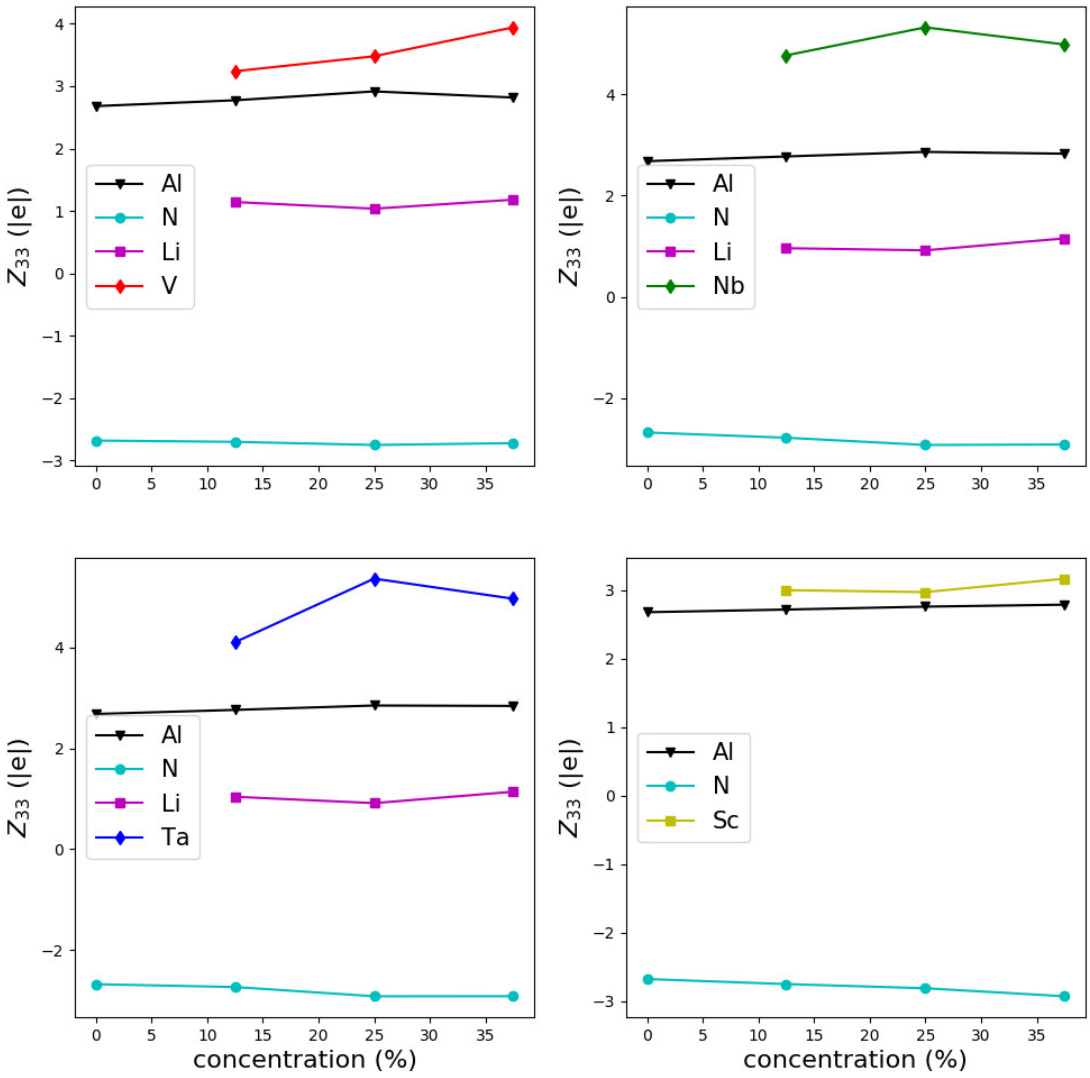


Figure S.1: The average Born effective charges Z_{33} of each atoms in (a) $Li_{x/2}V_{x/2}Al_{1-x}N$, (b) $Li_{x/2}Nb_{x/2}Al_{1-x}N$, (c) $Li_{x/2}Ta_{x/2}Al_{1-x}N$, and (d) $Sc_xAl_{1-x}N$ (x=0-0.375).

The average $\frac{du_3}{d\eta_3}$ of each atoms

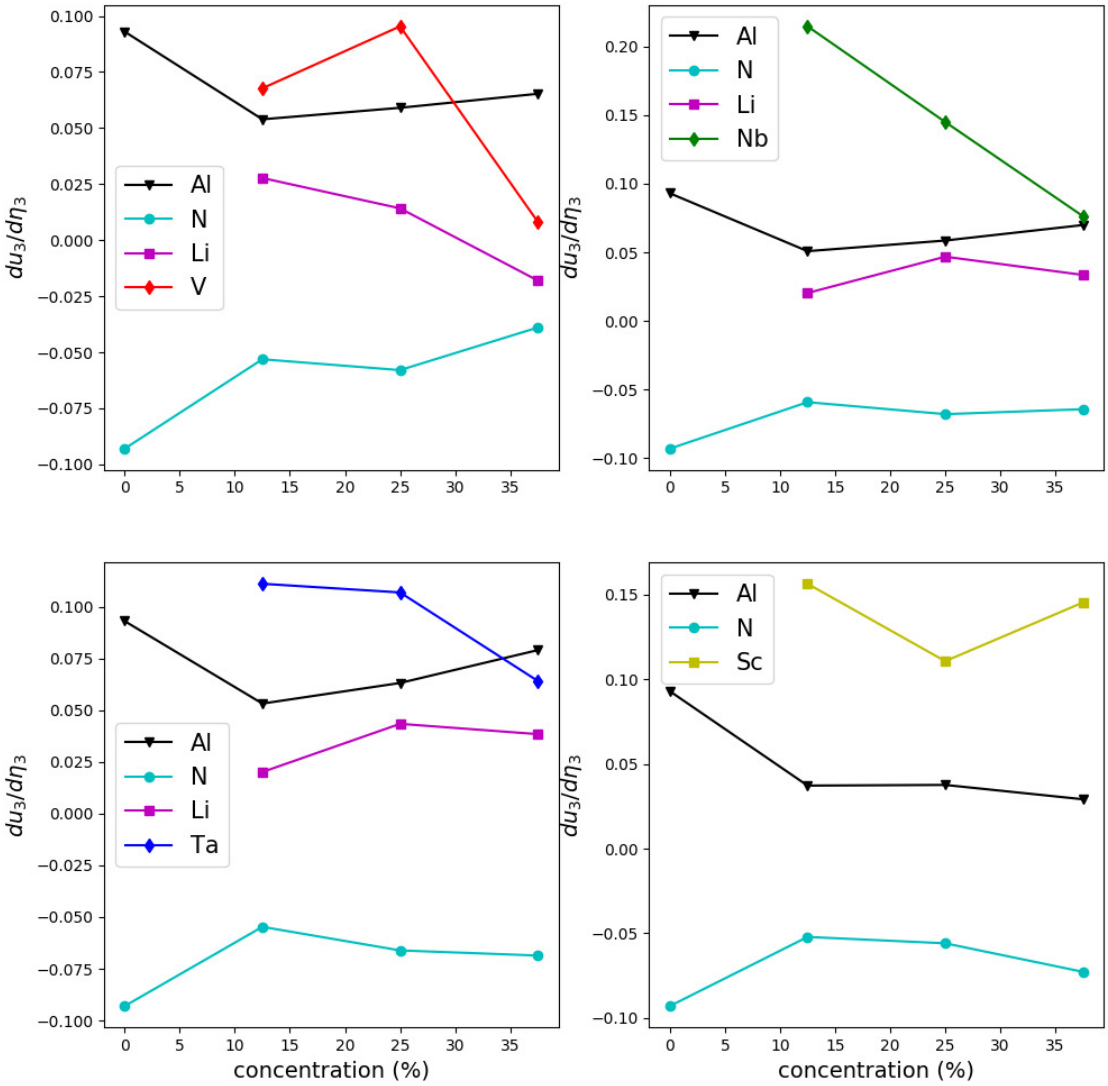


Figure S.2: The average $\frac{du_3}{d\eta_3}$ – the response of the internal coordinate along the c-direction (u_3) to a macroscopic strain (η_3) – of each atoms in (a) $Li_{x/2}V_{x/2}Al_{1-x}N$, (b) $Li_{x/2}Nb_{x/2}Al_{1-x}N$, (c) $Li_{x/2}Ta_{x/2}Al_{1-x}N$, and (d) $Sc_xAl_{1-x}N$ (x=0-0.375).

The optimized structures

$Li_{0.0625}V_{0.0625}Al_{0.8750}N$

1.00000000000000

6.2939611484099256 -0.0033083099091922 0.0048438204818929

-3.1498456546299152 5.4556927098190631 0.0000000000000000

0.0076411669642681 0.0044116298037431 9.9968677820038945

Al N Li V

14 16 1 1

Direct

0.1657683901572145 0.3325405161760037 0.9933545085748363

0.6681733299741662 0.3340866649870867 0.9973640845235250

0.1657683901572145 0.8332278739812180 0.9933545085748789

0.6678534239919699 0.8339267119959886 0.9859383115762100

0.1568526884851728 0.3220246043381142 0.4980573290317258

0.6745616309387718 0.3372808154693894 0.4995712431719491

0.1568526884851728 0.8348280841470659 0.4980573290317471

0.3355948505552850 0.1677974252776390 0.7456943417641740

0.8314612191856331 0.1638239675425310 0.7456052302404079

0.3376249533774306 0.6688124766887116 0.7477529483936636

0.8314612191856331 0.6676372516430951 0.7456052302403724

0.3407171890951390 0.1703585945475660 0.2528247291493746

0.8281058855350300 0.1676143342304107 0.2567810346226143

0.8281058855350300 0.6604915513046120 0.2567810346225930

0.1682833404906117 0.3335272321731209 0.1892236938227253

0.6656662199126282 0.3328331099563177 0.1883160106455068

0.1682833404906117 0.8347561083174980 0.1892236938228958

0.6655610406776669 0.8327805203388373 0.1873781753247200

0.1691279401901507 0.3361703475565327 0.6889853659269788

0.6675856221020370 0.3337928110510220 0.6918206933821918

0.1691279401901507 0.8329575926336252 0.6889853659270143

0.6663129766388929 0.8331564883194502 0.7078531648587499

0.3330315785557749 0.1665157892778839 0.9396906684510099

0.8359229391902384 0.1706160199265656 0.9415614792704023

0.3292108119320711 0.6646054059660322 0.9429587300307808

0.8359229391902384 0.6653069192636659 0.9415614792703668

0.3350827130487510 0.1675413565243720 0.4404300876569461

0.8393705162823533 0.1798651910394972 0.4389559379823929

0.3135940855474786 0.6567970427737359 0.4188229352706418

0.8393705162823533 0.6595053252428489 0.4389559379822365

0.6773701343185446 0.8386850671592759 0.5039889545649699

0.3322736003005832 0.6661368001502881 0.2445457622913916

Elastic co-efficient: C_{11}= 340.29 GPa, C_{12}= 126.49 GPa, C_{33}= 292.90 GPa, C_{44}= 106.50 GPa

Piezoelectric co-efficient: d_{31}= -3.007 pC/N, d_{32}= -2.977 pC/N, d_{33}= 8.550 pC/N

$Li_{0.0625}V_{0.0625}Al_{0.8750}N$ (Li and V positions are swapped)

1.00000000000000

6.3081340234826087 -0.0000000000000000 -0.0000000000000000

-3.1540670117413043 5.4630043148128813 0.0000000000000000

0.0000000000000000 0.0000000000000000 9.9687147647682366

Al N Li V

14 16 1 1

Direct

0.1688245963887062 0.3311754036112938 -0.0052272989865973

0.6623503072225818 0.3311754036112938 -0.0052272989865973

0.1688245963887062 0.8376496927774182 -0.0052272989865973

0.6666664999999981 0.8333335000000019 -0.0047636060574524

0.1722914935122868 0.3277085064877131 0.5067592532931459

0.6554165129754204 0.3277085064877131 0.5067592532931459

0.1722914935122868 0.8445834870245796 0.5067592532931459

0.8414816398683538 0.1829627797367011 0.7473524432011321

0.3170372202632991 0.6585183601316462 0.7473524432011321

0.8414816398683538 0.6585183601316462 0.7473524432011321

0.3333335000000019 0.1666664999999981 0.2395187867472466

0.8338154242075824 0.1676303484151586 0.2419414237977029

0.3323696515848414 0.6661845757924176 0.2419414237977029

0.8338154242075824 0.6661845757924176 0.2419414237977029

0.1643405405399125 0.3356594594600876 0.1921380789935864

0.6713184189201693 0.3356594594600876 0.1921380789935864

0.1643405405399125 0.8286815810798307 0.1921380789935864

0.6666664999999981 0.8333335000000019 0.1895519164133699

0.1607897405906583 0.3392102594093418 0.6882419642522986

0.6784200188186778 0.3392102594093418 0.6882419642522986

0.1607897405906583 0.8215799811813222 0.6882419642522986

0.6666664999999981 0.8333335000000019 0.6784725952088971

0.3333335000000019 0.1666664999999981 0.9606064763053729

0.8325733059969481 0.1651461119938901 0.9396355821072170

0.3348538880061100 0.6674266940030519 0.9396355821072170

0.8325733059969481 0.6674266940030519 0.9396355821072170

0.3333335000000019 0.1666664999999981 0.4350379545036310

0.8298515450060215 0.1597025900120371 0.4395470686463785

0.3402974099879628 0.6701484549939785 0.4395470686463785

0.8298515450060215 0.6701484549939785 0.4395470686463785

0.3333335000000019 0.1666664999999981 0.7546404037485610

0.6666664999999981 0.8333335000000019 0.4957699272157816

Elastic co-efficient: C_{11}= 336.87 GPa, C_{12}= 122.84 GPa, C_{33}= 277.12 GPa, C_{44}= 106.53 GPa

Piezoelectric co-efficient: d_{31}= -3.197 pC/N, d_{32}= -3.179 pC/N, d_{33}= 9.179 pC/N

$\mathbf{Li_{0.125}V_{0.125}Al_{0.750}N}$

1.00000000000000

6.3100583718652139 0.0000000000000000 0.0000000000000000

-3.1550291859326069 5.5120437906683453 0.0031714110051273

0.0000000000000000 0.0058046133677807 9.9250406100949906

Al N Li V

12 16 2 2

Direct

0.1614391304039627 0.3354117099570164 0.9941194797403023

0.6739725795530461 0.3354117099570164 0.9941194797403023

0.1624375439588895 0.8248750879177860 0.9958715573463905

0.6680865882234515 0.8361731764469101 0.9992552515873737

0.1598307587465741 0.8196615174931552 0.4885126858499068

0.6708041787092195 0.8416083574184463 0.4947258706423611

0.8300930028455299 0.1601860056910524 0.7373142012002697

0.3418172478403116 0.6703079307306844 0.7451176780681421

0.8284906828903802 0.6703079307306844 0.7451176780681421

0.8320085740252282 0.1640171480504493 0.2679577914979033

0.3398209484576825 0.6676612088222358 0.2577725685688255

0.8278402603645598 0.6676612088222358 0.2577725685688255

0.1659986105265834 0.3354705094858438 0.1879698754633118

0.6694718989592533 0.3354705094858438 0.1879698754633118

0.1648382738851711 0.8296765477703492 0.1870881003798368

0.6677572220312227 0.8355144440624525 0.1892537737202648

0.1767976992847608 0.3305886993702562 0.7080703559567217

0.6537910000854883 0.3305886993702562 0.7080703559567217

0.1691135231644837 0.8382270463289744 0.6911194520088831

0.6662362623422705 0.8324725246845480 0.6921463125172506

0.3315438613240657 0.1630877226481245 0.9401530735990689

0.8326268430315149 0.1652536860630224 0.9355867458188577

0.3333297113121256 0.6669133304813969 0.9383796073954868

0.8335836191692784 0.6669133304813969 0.9383796073954868

0.3222041307612541 0.1444082615225008 0.4129550460205320

0.8297879098728977 0.1595758197457887 0.4494686069517846

0.3428254387993956 0.6812493272162429 0.4424128130491751

0.8384238884168542 0.6812493272162429 0.4424128130491751

0.1670073129574578 0.3394670759910636 0.4901088037013570

0.6724597630335986 0.3394670759910636 0.4901088037013570

0.3339552862563976 0.1679105725127882 0.7462744637610660

0.3316062487670899 0.1632124975341726 0.2444147032116204

Elastic co-efficient: C_{11}= 317.57 GPa, C_{12}= 119.66 GPa, C_{33}= 183.16 GPa, C_{44}= 91.12 GPa

Piezoelectric co-efficient: d_{31}= -5.319 pC/N, d_{32}= -5.645 pC/N, d_{33}= 19.587 pC/N

$Li_{0.125}V_{0.125}Al_{0.750}N$ (Li and V positions are swapped)

1.00000000000000

6.3556978736701231 0.0000000000000000 0.0000000000000000

-3.1778489368350615 5.5030709410687102 0.0149303906929321

0.0000000000000000 0.0266086060174102 9.8653881615556198

Al N Li V

12 16 2 2

Direct

0.1715773387006829 0.3295516045346212 0.0054051704316973

0.6579742658339310 0.3295516045346212 0.0054051704316973

0.1702664605584132 0.8405329211168330 0.0035100104921234

0.6658923733311042 0.8317847466622148 0.9970613353333601

0.1645637280436965 0.8291274560874001 0.5023904664193254

0.6631609738975217 0.8263219477950509 0.5013182140401076

0.8315075755403691 0.1630151510807314 0.7491633519444938

0.3323586077272521 0.6766893053196983 0.7519542679244990

0.8443306975924536 0.6766893053196983 0.7519542679244990

0.8345705687908230 0.1691411375816388 0.2361739754899564

0.3272410013018852 0.6635606588807261 0.2376936417239750

0.8363196575788477 0.6635606588807261 0.2376936417239750

0.1583708938448216 0.3387027050970332 0.1966844343043215

0.6803318112522043 0.3387027050970332 0.1966844343043215

0.1598261742151922 0.8196523484303917 0.1947183440644603

0.6662288978467830 0.8324577956935733 0.1925753540921118

0.1546993635180370 0.3489600960907124 0.6703547191398591

0.6942607325726683 0.3489600960907124 0.6703547191398591

0.1586250491441514 0.8172500982883101 0.6874029570710308

0.6665406371970668 0.8330812743941406 0.6906647796030342

0.3340558543457999 0.1681117086915926 0.9504976715202179

0.8341155658957535 0.1682311317914999 0.9386799398449407

0.3329676750468386 0.6646783645504354 0.9419620981944039

0.8317106895036036 0.6646783645504354 0.9419620981944039

0.3353230344231917 0.1706460688463764 0.4558355078929872

0.8296892227316004 0.1593784454631939 0.4428318713460252

0.3353042398276159 0.6660767529789412 0.4410064450466943

0.8307725131513325 0.6660767529789412 0.4410064450466943

0.3293848859175948 0.1587697718351826 0.7500865753816157

0.3323381237928523 0.1646762475856974 0.2337248104593243

0.1685146530580099 0.3356913868759190 0.4916216407369996

0.6671767338179019 0.3356913868759190 0.4916216407369996

Elastic co-efficient: C_{11}= 313.89 GPa, C_{12}= 121.81 GPa, C_{33}= 209.04 GPa, C_{44}= 89.03 GPa

Piezoelectric co-efficient: d_{31}= -4.985 pC/N, d_{32}= -4.611 pC/N, d_{33}= 16.702 pC/N

$\mathbf{Li_{0.1875}V_{0.1875}Al_{0.6250}N}$

1.00000000000000

6.3903243311169238 -0.0465982443445125 0.0035485456122222

-3.2359339513484535 5.5157714373735134 -0.0222333879226922

0.0096340587581447 -0.0412165512412066 9.9689203425447097

Al N Li V

10 16 3 3

Direct

0.1626367463172171 0.3218208441489797 -0.0059431965816178

0.6678373853088161 0.3430424090783790 -0.0001984226997751

0.1523430080457800 0.8361067569811014 -0.0040109045698561

0.6690049267498089 0.3408560841719928 0.4956357857924109

0.1591776024433547 0.8275234779353827 0.5054732254021179

0.6682397827789216 0.8282416755943182 0.4942277745812178

0.3317272846129909 0.1532375818138844 0.7486939424573179

0.8422084216070111 0.6729194619003888 0.7546881226735905

0.3438420056645902 0.1715799754905077 0.2439047129445645

0.8264054002666086 0.6561593217285049 0.2466314371161699

0.1812628969989711 0.3304560732054583 0.1868969895729552

0.6625990612912896 0.3364028992406940 0.1871235970110636

0.1596645985960373 0.8409262814959010 0.1933224581795729

0.6466707402779917 0.8098314682552146 0.2131686273441458

0.1651946547327876 0.3160312429238532 0.6842349779160845

0.6629584747696087 0.3332051054720420 0.6872769811366986

0.1589099599443274 0.8374701432535280 0.6897913943304148

0.6912933834787047 0.8495742247866216 0.6889222617365630

0.3326849912480139 0.1667924493890371 0.9373706111365568

0.8455363559634390 0.1902883922348915 0.9180564277511151

0.3194370456303623 0.6634492681155287 0.9873949198513883

0.8369399141921621 0.6592564274217673 0.9382026408245457

0.3320948254641513 0.1673260389587208 0.4415937195285120

0.8406182867369215 0.1746070200335579 0.4609031554663505

0.3237459092292318 0.6543696394689958 0.4583379899104033

0.8333045930122922 0.6659496013115529 0.4405982253644588

0.6793454662331242 0.8397996469442116 -0.0070088166481476

0.3377685785060263 0.6788431590089433 0.7593059579159201

0.8300231665051414 0.1689219160102367 0.2431546557951683

0.1655391014649433 0.3334994862355657 0.4960812349978847

0.8343713809358397 0.1673240247820351 0.7382589108000095

0.3366140509935334 0.6641879026082019 0.1779106029621955

Elastic co-efficient: C_{11}= 278.02 GPa, C_{12}= 119.93 GPa, C_{33}= 157.29 GPa, C_{44}= 85.79 GPa

Piezoelectric co-efficient: d_{31}= -4.657 pC/N, d_{32}= -4.432 pC/N, d_{33}= 13.599 pC/N

$\mathbf{Li_{0.1875}V_{0.1875}Al_{0.6250}N}$ (Li and V positions are swapped)

1.00000000000000

6.3946198246987240 -0.0442978748425683 0.0229490209525122

-3.2353384274343422 5.5111527366868778 -0.0041698090118623

0.0378840493147539 0.0122851812046708 9.9655614527968712

Al N Li V

10 16 3 3

Direct

0.1717522451357678 0.3317899339286900 -0.0058289332445614

0.6591215435518856 0.3309931050170250 -0.0044058154512066

0.1725043772955110 0.8408430177704290 0.0054583907784747

0.6569731129286834 0.3321612234037266 0.4998097713006063

0.1638918846053457 0.8476682471878926 0.4959554676611018

0.6781595682943211 0.8373691826369692 0.4940693676172473

0.3438192284439259 0.1735717138444820 0.7466039768873161

0.8284328557479431 0.6561108232260537 0.7439227962964440

0.3270816188726532 0.1577986551441625 0.2546594007970899

0.8467830199317360 0.6682921366857008 0.2486703202011843

0.1504416953680858 0.3087638409402183 0.1889229434969715

0.6668091874373914 0.3370523231553060 0.1872891770237400

0.1625571007445019 0.8411054164796707 0.1898243695608957

0.6839528333565766 0.8348279449009214 0.1842159551610193

0.1901564427653636 0.3533247484640591 0.7131619315459091

0.6636035859772507 0.3373666138991467 0.6871744132095876

0.1590719629040364 0.8403041850405828 0.6933481721217716

0.6695478049296556 0.8187057916720303 0.6869782608806217

0.3340004200403170 0.1666701614932423 0.9406082363201808

0.8253646283665400 0.1593557575985352 0.9608944550460474

0.3456291648192419 0.6762555389989612 0.9582618243804949

0.8326748358616151 0.6679079634093895 0.9416139977466577

0.3407809999154545 0.1630892464799137 0.4382267748132471

0.8097346786856879 0.1544655583591426 0.4180991247079219

0.3365668781804688 0.6806037867132660 0.4873685176930955

0.8332079373257903 0.6673212224640507 0.4374032803026807

0.1602115069918567 0.3206915894769545 0.4929441492274285

0.8310766058417293 0.1699502212681465 0.7431318875687866

0.3211500064706048 0.6622144184619503 0.2593864481762528

0.6664631211929608 0.8344289261534514 -0.0039679909430733

0.3358025371907951 0.6633690632754645 0.6779624579683740

0.8326766108263053 0.1656276424504632 0.2382368711476927

Elastic co-efficient: C_{11}= 282.84 GPa, C_{12}= 121.92 GPa, C_{33}= 158.63 GPa, C_{44}= 85.25 GPa

Piezoelectric co-efficient: d_{31}= -3.734 pC/N, d_{32}= -5.429 pC/N, d_{33}= 13.718 pC/N

$\mathbf{Li_{0.0625}Nb_{0.0625}Al_{0.8750}N}$

1.00000000000000

6.3391339146832726 -0.0036376732969229 -0.0030170085944349

-3.1727172748274399 5.4953075180525950 -0.0000000000000000

-0.0047755441074077 -0.0027571616759388 10.0146138265106757

Al N Li Nb

14 16 1 1

Direct

0.1640670734662727 0.3287433342578081 0.9901954014788820

0.6680642926275774 0.3340321463137922 0.9967702984362937

0.1640670734662727 0.8353237392084717 0.9901954014789246

0.6718919451052068 0.8359459725526071 0.9807699147779532

0.1559655547251706 0.3229008193823407 0.5005378496824137

0.6740459977594562 0.3370229988797316 0.4978493490821019

0.1559655547251706 0.8330647353428369 0.5005378496824350

0.3356948523271287 0.1678474261635608 0.7450521393379934

0.8296423809828439 0.1639450981509388 0.7452883169039604

0.3355709518981976 0.6677854759490955 0.7477471793238595

0.8296423809828439 0.6656972828318982 0.7452883169039248

0.3393107419583138 0.1696553709791534 0.2528779365750681

0.8313347367166033 0.1679325114298204 0.2559246473690486

0.8313347367166033 0.6634022252867759 0.2559246473690273

0.1621308744457472 0.3189977747905092 0.1854383396521137

0.6656300007296957 0.3328150003648514 0.1886172203218428

0.1621308744457472 0.8431330996552453 0.1854383396522842

0.6836840682051039 0.8418420341025556 0.1827131381923367

0.1669596047380212 0.3342254514203076 0.6915501017040784

0.6663683136023695 0.3331841568011883 0.6902737152848457

0.1669596047380212 0.8327341533177209 0.6915501017041139

0.6647297607572646 0.8323648803786359 0.7120963163216347

0.3344402339345055 0.1672201169672492 0.9380207994220138

0.8353463145711547 0.1722460675742129 0.9400365016519678

0.3290353513619744 0.6645176756809839 0.9465800329186327

0.8353463145711547 0.6631002469969348 0.9400365016519323

0.3329840908141601 0.1664920454070765 0.4408900495628074

0.8398291015195474 0.1806563423975592 0.4382256739763886

0.3157840803740437 0.6578920401870181 0.4343155827075381

0.8398291015195474 0.6591727591219811 0.4382256739762322

0.6765116227015250 0.8382558113507661 0.5060558975293633

0.3357024135127546 0.6678512067563739 0.2449767653679818

Elastic co-efficient: C_{11}= 333.96 GPa, C_{12}= 125.63 GPa, C_{33}= 276.87 GPa, C_{44}= 103.72 GPa

Piezoelectric co-efficient: d_{31}= -3.681 pC/N, d_{32}= -3.607 pC/N, d_{33}= 9.731 pC/N

$Li_{0.0625}Nb_{0.0625}Al_{0.8750}N$ (Li and Nb positions are swapped)

1.00000000000000

6.3553606906522644 -0.0140871938260664 -0.0063923394801468

-3.1898802130475410 5.5250345990569745 -0.0000000000000000

-0.0105044727130941 -0.0060647601485999 9.8858316224162301

Al N Li Nb

14 16 1 1

Direct

0.1699476603035137 0.3343879829300038 0.0017620773692425

0.6646099048294065 0.3323049524147068 -0.0036544080249392

0.1699476603035137 0.8355596773735169 0.0017620773692425

0.6638907214627137 0.8319453607313602 0.0110316510596244

0.1664239070433306 0.3293324191359517 0.4985413129043079

0.6592379116534937 0.3296189558267504 0.5004933258023170

0.1664239070433306 0.8370914879073856 0.4985413129043079

0.3316291507810430 0.1658145753905179 0.7495715419748958

0.8332870912492801 0.1657592030176272 0.7504227608095968

0.3328224075589626 0.6664112037794776 0.7476868034948096

0.8332870912492801 0.6675278882316457 0.7504227608095968

0.3288555094763716 0.1644277547381822 0.2415912696087284

0.8471158721911852 0.1804531454467761 0.2356120087812073

0.8471158721911852 0.6666627267444020 0.2356120087812073

0.1661147425456153 0.3225745215917399 0.1881579536504673

0.6676078020735472 0.3338039010367772 0.1888581070171944

0.1661147425456153 0.8435402209538823 0.1881579536504673

0.6838895439259693 0.8419447719629880 0.2100043883946157

0.1646830842655893 0.3313863019500946 0.6906835415630835

0.6671060522026574 0.3335530261013323 0.6913701117906551

0.1646830842655893 0.8332967823155017 0.6906835415630835

0.6690928424831591 0.8345464212415830 0.6804355636503487

0.3340507578969348 0.1670253789484638 0.9386849465635936

0.8301035174205452 0.1622617079736465 0.9424219682397242

0.3368381985499948 0.6684190992749939 0.9401366183716917

0.8301035174205452 0.6678418094468919 0.9424219682397242

0.3311673221118631 0.1655836610559280 0.4414746314820916

0.8390693451394132 0.1871619815798511 0.4376695007321332

0.3134738340110820 0.6567369170055375 0.4521959234945404

0.8390693451394132 0.6519073635595551 0.4376695007321332

0.3227425633110435 0.6613712816555180 0.2366148415774069

0.6594950373548122 0.8297475186774091 0.4629624356428910

Elastic co-efficient: C_{11}= 338.91 GPa, C_{12}= 132.77 GPa, C_{33}= 253.07 GPa, C_{44}= 102.09 GPa

Piezoelectric co-efficient: d_{31}= -4.542 pC/N, d_{32}= -5.207 pC/N, d_{33}= 16.009 pC/N

$\mathbf{Li_{0.125}Nb_{0.125}Al_{0.750}N}$

1.00000000000000

6.3766857288803651 0.0000000000000000 0.0000000000000000

-3.1883428644401826 5.6031209305772176 -0.0067135515809966

0.0000000000000000 -0.0112287360256809 9.8800146407503906

Al N Li Nb

12 16 2 2

Direct

0.1668828999500273 0.3326572635258179 0.9895513730204499

0.6657743635757835 0.3326572635258179 0.9895513730204499

0.1674675870573460 0.8349351741146991 0.9927144333650314

0.6680179620872033 0.8360359241744139 0.9967103118944363

0.1475716587986662 0.7951433175973392 0.4925911039412313

0.6694718875850392 0.8389437751700846 0.4912808161270783

0.8317286520087159 0.1634573040174246 0.7434981130880498

0.3406918347678023 0.6707067810268973 0.7487026649409011

0.8300149462591023 0.6707067810268973 0.7487026649409011

0.8308263042914663 0.1616526085829263 0.2585037433748037

0.3414430630959068 0.6702489985593489 0.2522895946849676

0.8288059354634493 0.6702489985593489 0.2522895946849676

0.1678717115624977 0.3388131195615185 0.1878621371839232

0.6709414079990136 0.3388131195615185 0.1878621371839232

0.1664484598765968 0.8328969197532010 0.1894585527587499

0.6672692855706356 0.8345385711412779 0.1861743615520344

0.1637626391847058 0.3463721987132525 0.7043686790110085

0.6826095595285394 0.3463721987132525 0.7043686790110085

0.1550828527586549 0.8101657055173173 0.6903371006168836

0.6677195530446944 0.8354391060893962 0.6930922822584338

0.3308486804175647 0.1616973608351228 0.9337954240248328

0.8326666469660908 0.1653332939321746 0.9397108843401163

0.3333987048664772 0.6675895648989466 0.9416809021283118

0.8341908600324769 0.6675895648989466 0.9416809021283118

0.3221999422201413 0.1443998844402753 0.4672785903430426

0.8243207712105685 0.1486415424211290 0.4385535109995812

0.3428092312478404 0.6779841629790360 0.4373047720439098

0.8351749317312026 0.6779841629790360 0.4373047720439098

0.1473634534297101 0.3447550486794241 0.4935283251464105

0.6973915952497070 0.3447550486794241 0.4935283251464105

0.3355904997910382 0.1711809995820691 0.7034666956245460

0.3336421183713363 0.1672842367426652 0.2722571793713979

Elastic co-efficient: C_{11}= 302.97 GPa, C_{12}= 116.09 GPa, C_{33}= 229.49 GPa, C_{44}= 84.67 GPa

Piezoelectric co-efficient: d_{31}= -4.514 pC/N, d_{32}= -3.974 pC/N, d_{33}= 13.954 pC/N

$Li_{0.125}Nb_{0.125}Al_{0.750}N$ (Li and Nb positions are swapped)

1.00000000000000

6.4892448972899555 0.0000000000000000 0.0000000000000000

-3.2446224486449777 5.6141479248286403 -0.0129943147840679

0.0000000000000000 -0.0230301233912500 9.7658337215270095

Al N Li Nb

12 16 2 2

Direct

0.1745339085363142 0.3335686979388179 0.0087060058397270

0.6590347894024964 0.3335686979388179 0.0087060058397270

0.1706589888632375 0.8413179777264819 0.0003539585622376

0.6650249739020704 0.8300499478041479 -0.0066164966806076

0.1632627838504511 0.8265255677009092 0.5069779695908297

0.6632172543604866 0.8264345087209806 0.5051568543262954

0.8338264413396996 0.1676528826793920 0.7528696788030382

0.3273134428757444 0.6689201142308848 0.7518617798476088

0.8416066713551476 0.6689201142308848 0.7518617798476088

0.8325117886438040 0.1650235772876013 0.2274551791489684

0.3325589746471655 0.6768313197359417 0.2348815267006594

0.8442723450887829 0.6768313197359417 0.2348815267006594

0.1600716361338745 0.3459600238044168 0.2080452622447546

0.6858883876705351 0.3459600238044168 0.2080452622447546

0.1593106261263337 0.8186212522526747 0.1909672251617817

0.6664931735142898 0.8329863470285865 0.1887735038347831

0.1508467902021453 0.3453283086070916 0.6757237829898030

0.6944815184049390 0.3453283086070916 0.6757237829898030

0.1566571494026605 0.8133142988053282 0.6933239350467211

0.6665149571028912 0.8330299142057901 0.6963821224075312

0.3357738018259324 0.1715476036518575 0.9600712832863001

0.8349264917934374 0.1698529835868679 0.9477404170636194

0.3326848884883831 0.6633249291284871 0.9449166915900262

0.8306400406401113 0.6633249291284871 0.9449166915900262

0.3216244251439763 0.1432488502879454 0.4466105326482998

0.8179723565469573 0.1359447130939077 0.4335305192500957

0.3462358791736229 0.6855359362337419 0.4390469138950147

0.8393000570601257 0.6855359362337419 0.4390469138950147

0.3297539321704422 0.1595078643408771 0.7537670386588423

0.3302760412288940 0.1605520824577807 0.2228244131010304

0.1671542392621879 0.3327254845050536 0.4767239697875229

0.6655712452428586 0.3327254845050536 0.4767239697875229

Elastic co-efficient: C_{11}= 303.28 GPa, C_{12}= 123.16 GPa, C_{33}= 180.86 GPa, C_{44}= 81.87 GPa

Piezoelectric co-efficient: d_{31}= -8.087 pC/N, d_{32}= -7.992 pC/N, d_{33}= 27.907 pC/N

$\mathbf{Li_{0.1875}Nb_{0.1875}Al_{0.6250}N}$

1.00000000000000

6.5606420793537055 -0.0919789450773587 0.0002888789199298

-3.3596260378568359 5.6795785479447485 -0.0080599718422737

0.0020088641246385 -0.0164509184314067 9.8475933212061673

Al N Li Nb

10 16 3 3

Direct

0.1599739512167940 0.3176354080453480 0.0030848401952703

0.6713664252005487 0.3447839727925868 -0.0004825873992221

0.1528885217027131 0.8299996864556897 -0.0092089885213084

0.6652091562455589 0.3416683867504376 0.4929471553632025

0.1615130524176334 0.8310461628161269 0.5059647183354063

0.6650496029992994 0.8257464233858114 0.4875126604781573

0.3285506809073394 0.1569068884777566 0.7492705212419370

0.8378645542484596 0.6712964631646769 0.7513330865131869

0.3507394206689278 0.1700302408665714 0.2405075182499792

0.8332103574885040 0.6648985847516194 0.2445938253249806

0.1790075085996075 0.3209867541106414 0.2099103295640781

0.6667975372560153 0.3468489125266266 0.1895710215886182

0.1593192134653178 0.8521348273769562 0.1903351791512827

0.6783317443622811 0.8301758552368715 0.2163099444559022

0.1762429832530243 0.3177643115840666 0.6783435828673514

0.6548039122394875 0.3379411196611912 0.6868838104466694

0.1596452335897413 0.8411212833596213 0.6932226813105556

0.6794827747651161 0.8278581179598183 0.6841301796075545

0.3300159497413965 0.1667669303203898 0.9425971785821049

0.8440494880501672 0.1866375535979639 0.9339451136251085

0.3101105630365634 0.6518556498304032 0.9892212276115794

0.8380610505808637 0.6555761408604635 0.9376777659625694

0.3397689706977025 0.1560220789096200 0.4381219166174178

0.8167993688643496 0.1652604386901509 0.4641088481773358

0.3292701307546795 0.6790333424427538 0.4415831508615106

0.8344336016190167 0.6663450729219652 0.4416316919943984

0.6791151428345227 0.8303090305304988 -0.0071620874373714

0.3342469333765275 0.6711357149595732 0.7617108791352494

0.8236042279837003 0.1707337378104856 0.2370934105267517

0.1643703969249094 0.3321077341771577 0.4710099935414267

0.8309866122940650 0.1629025479989223 0.7354897422943927

0.3451709326151668 0.6764706276272340 0.1987416897339242

Elastic co-efficient: C_{11}= 267.97 GPa, C_{12}= 128.40 GPa, C_{33}= 166.11 GPa, C_{44}= 77.82 GPa

Piezoelectric co-efficient: d_{31}= -6.198 pC/N, d_{32}= -8.381 pC/N, d_{33}= 24.182 pC/N

$\mathbf{Li_{0.1875}Nb_{0.1875}Al_{0.6250}N}$ (Li and Nb positions are swapped)

1.00000000000000

6.6024649438037333 -0.0708702960690094 0.0087529865846012

-3.3629643088387748 5.6377135641885561 -0.0003563562377678

0.0141828482852877 0.0067342844230026 9.8451679610961929

Al N Li Nb

10 16 3 3

Direct

0.1742725835494938 0.3349389056553955 -0.0125572494017538

0.6583435452049730 0.3347792836166044 -0.0071088654937550

0.1689339327642749 0.8385094168232002 0.0059382130565902

0.6552064464799136 0.3285808280386798 0.4995074318361628

0.1700190897232301 0.8470869254948189 0.4907501602587999

0.6822834453437806 0.8399300897650502 0.5030910511267395

0.3351340689498346 0.1668074075786740 0.7445504094804835

0.8299778829830275 0.6493252231764096 0.7404828611733800

0.3287232216660185 0.1621190991587050 0.2513359741776538

0.8430487870940778 0.6714250755889759 0.2492479641438939

0.1721148400167942 0.3204333853699790 0.1841087665854054

0.6620625951966131 0.3451204873490007 0.1869088797139591

0.1588062885858953 0.8403739288516486 0.1932801413988900

0.6823587545572777 0.8238236735692924 0.1783858579355129

0.1699488143175922 0.3217310402581237 0.7164126113355971

0.6531838757502448 0.3332315646246815 0.6896162677904416

0.1478863262987451 0.8406499979455192 0.6903690309727443

0.6789078608019514 0.8208587259493045 0.7098877981832266

0.3336583242444892 0.1655861630569967 0.9416397518321198

0.8347310932349806 0.1832319761116944 0.9641147777031236

0.3210114685160830 0.6708282200636754 0.9416465349394253

0.8439207324903923 0.6602707621352155 0.9381555347232386

0.3444318822461419 0.1619169128582179 0.4377350635302802

0.8132760212857185 0.1558878558670573 0.4339864326279225

0.3481162322816344 0.6899240018196334 0.4891962916396702

0.8331685556386937 0.6699652834142447 0.4426291299033402

0.1697810303954201 0.3209517637871179 0.4927613988461305

0.8293172710262048 0.1764435827114994 0.7369704954050454

0.3288175484983829 0.6657804361201253 0.2616900585182598

0.6678732560421898 0.8356267165151116 -0.0290022320103383

0.3235522523492693 0.6548178633793231 0.6987778236847902

0.8371319724666623 0.1690434033460248 0.2354916343830207

Elastic co-efficient: C_{11}= 273.30 GPa, C_{12}= 129.62 GPa, C_{33}= 167.26 GPa, C_{44}= 79.17 GPa

Piezoelectric co-efficient: d_{31}= -7.0189 pC/N, d_{32}= -7.506 pC/N, d_{33}= 24.011 pC/N

$\mathbf{Li_{0.0625}Ta_{0.0625}Al_{0.8750}N}$

1.00000000000000

6.3390729013754701 -0.0025921422114463 -0.0017817318460848

-3.1717813116930689 5.4936863823498543 0.0000000000000000

-0.0028306351410808 -0.0016342679606806 10.0069254443308271

Al N Li Ta

14 16 1 1

Direct

0.1638403727570492 0.3283686518418677 0.9900138489388549

0.6680161599367346 0.3340080799683708 0.9967518434683013

0.1638403727570492 0.8354717209151886 0.9900138489388975

0.6720466062388601 0.8360233031194337 0.9801591043940271

0.1568462525166184 0.3245829626016863 0.5002659180165424

0.6739797097386115 0.3369898548693093 0.4977297780552609

0.1568462525166184 0.8322632899149391 0.5002659180165637

0.3356040632584130 0.1678020316292030 0.7448674146716876

0.8298264335546033 0.1641604755250733 0.7451211325062385

0.3355029134441914 0.6677514567220925 0.7476892200957586

0.8298264335546033 0.6656659580295226 0.7451211325062029

0.3391028600513978 0.1695514300256953 0.2529971825800613

0.8311438910474205 0.1676958002148890 0.2561495872476253

0.8311438910474205 0.6634480908325238 0.2561495872476039

0.1628157264430737 0.3205627641713432 0.1855968919989845

0.6654948585112079 0.3327474292556075 0.1886697717878016

0.1628157264430737 0.8422529622717375 0.1855968919991550

0.6818204917390112 0.8409102458695095 0.1830931102657082

0.1670658467239070 0.3343951179553778 0.6917067952594580

0.6663020095736305 0.3331510047868188 0.6903339575109613

0.1670658467239070 0.8326707287685364 0.6917067952594935

0.6647131211812126 0.8323565605906097 0.7128024044938054

0.3344453264412405 0.1672226632206167 0.9381066341639216

0.8354182749507792 0.1723582589755758 0.9401584606646471

0.3289627641823720 0.6644813820911825 0.9472684808359156

0.8354182749507792 0.6630600159751961 0.9401584606646116

0.3329272391115841 0.1664636195557885 0.4409412982432590

0.8400422133357041 0.1806547507620430 0.4384370557014300

0.3162418476901823 0.6581209238450877 0.4337638221119816

0.8400422133357041 0.6593874625736537 0.4384370557012737

0.6754309975852578 0.8377154987926327 0.5059763202966815

0.3354110086577831 0.6677055043288881 0.2439502763572777

Elastic co-efficient: C_{11}= 336.44 GPa, C_{12}= 126.07 GPa, C_{33}= 273.94 GPa, C_{44}= 104.89 GPa

Piezoelectric co-efficient: d_{31}= -3.764 pC/N, d_{32}= -3.768 pC/N, d_{33}= 10.076 pC/N

$Li_{0.0625}Ta_{0.0625}Al_{0.8750}N$ (Li and Ta positions are swapped)

1.00000000000000

6.3441836723072456 0.0000000000000000 0.0000000000000000

-3.1720918361536228 5.4942242264925252 0.0000000000000000

0.0000000000000000 -0.0000000000000000 10.0143072013859307

Al N Li Ta

14 16 1 1

Direct

0.1697507989373880 0.3302492010626120 -0.0052177726317074

0.6604979021252181 0.3302492010626120 -0.0052177726317074

0.1697507989373880 0.8395020978747819 -0.0052177726317074

0.6666664999999981 0.8333335000000019 -0.0042635215080532

0.1703656905483083 0.3296343094516918 0.5067835904918679

0.6592681189033778 0.3296343094516918 0.5067835904918679

0.1703656905483083 0.8407318810966222 0.5067835904918679

0.8417058202093213 0.1834111404186365 0.7504935349413507

0.3165888595813636 0.6582941797906787 0.7504935349413507

0.8417058202093213 0.6582941797906787 0.7504935349413507

0.3333335000000019 0.1666664999999981 0.2398580066555641

0.8362331878189103 0.1724658756378151 0.2388067773215560

0.3275341243621850 0.6637668121810897 0.2388067773215560

0.8362331878189103 0.6637668121810897 0.2388067773215560

0.1652974955023821 0.3347025044976178 0.1901208690165732

0.6694045089952297 0.3347025044976178 0.1901208690165732

0.1652974955023821 0.8305954910047703 0.1901208690165732

0.6666664999999981 0.8333335000000019 0.1934832696958276

0.1597012843772042 0.3402987156227958 0.6883155353773454

0.6805969312455858 0.3402987156227958 0.6883155353773454

0.1597012843772042 0.8194030687544142 0.6883155353773454

0.6666664999999981 0.8333335000000019 0.6895427491853819

0.3333335000000019 0.1666664999999981 0.9583066328963806

0.8329269164609899 0.1658533329219740 0.9420977367978722

0.3341466670780260 0.6670730835390101 0.9420977367978722

0.8329269164609899 0.6670730835390101 0.9420977367978722

0.3333335000000019 0.1666664999999981 0.4362493677166928

0.8381065577644562 0.1762126155289066 0.4350208960815931

0.3237873844710935 0.6618934422355438 0.4350208960815931

0.8381065577644562 0.6618934422355438 0.4350208960815931

0.3333335000000019 0.1666664999999981 0.7534242036304603

0.6666664999999981 0.8333335000000019 0.4941357895383926

Elastic co-efficient: C_{11}= 330.17 GPa, C_{12}= 121.04 GPa, C_{33}= 267.70 GPa, C_{44}= 104.44 GPa

Piezoelectric co-efficient: d_{31}= -3.676 pC/N, d_{32}= -3.670 pC/N, d_{33}= 10.017 pC/N

$\mathbf{Li_{0.125}Ta_{0.125}Al_{0.750}N}$

1.00000000000000

6.3738542009308050 0.0000000000000000 0.0000000000000000

-3.1869271004654025 5.5990660174522464 -0.0075844119257342

0.0000000000000000 -0.0127351427526402 9.8541247624282207

Al N Li Ta

12 16 2 2

Direct

0.1674992273842668 0.3318412994116613 0.9881439297188659

0.6643420720273870 0.3318412994116613 0.9881439297188659

0.1681230149151656 0.8362460298303381 0.9919546952405847

0.6680348314276079 0.8360696628552228 0.9959853135365413

0.1471317484145790 0.7942634968291650 0.4932912157987061

0.6693392680981884 0.8386785361963833 0.4913420483733985

0.8324950396229689 0.1649900792459309 0.7435801290245596

0.3398246673486710 0.6697493034354771 0.7488624515385897

0.8299246360868131 0.6697493034354771 0.7488624515385897

0.8301861454139192 0.1603722908278311 0.2575396893402077

0.3418501704955847 0.6705110441283747 0.2516991100313878

0.8286608736327968 0.6705110441283747 0.2516991100313878

0.1699647427681019 0.3366392843022556 0.1883981340382492

0.6666745415341466 0.3366392843022556 0.1883981340382492

0.1688434794858497 0.8376869589717066 0.1902772234943914

0.6670136799515949 0.8340273599031970 0.1857488400767733

0.1636485391056473 0.3465285139064098 0.7044680791642228

0.6828799748007554 0.3465285139064098 0.7044680791642228

0.1556597393756285 0.8113194787512640 0.6910720996516256

0.6677753747822428 0.8355507495644932 0.6934421409019883

0.3305868875393205 0.1611737750786341 0.9308799004926668

0.8327302233439970 0.1654604466879877 0.9404733633930594

0.3331263427725684 0.6675231787433664 0.9424517583704836

0.8343968359708049 0.6675231787433664 0.9424517583704836

0.3226650006911320 0.1453300013822568 0.4721054470788556

0.8240438258678279 0.1480876517356491 0.4375847134711809

0.3424350669359175 0.6776375413417159 0.4369198845412297

0.8352024744058058 0.6776375413417159 0.4369198845412297

0.1451190922170790 0.3453615899772424 0.4948989096801771

0.7002424977601565 0.3453615899772424 0.4948989096801771

0.3354612143339605 0.1709224286679139 0.6989735655767521

0.3341187714895140 0.1682375429790208 0.2740651003823124

Elastic co-efficient: C_{11}= 310.23 GPa, C_{12}= 120.12 GPa, C_{33}= 237.70 GPa, C_{44}= 86.11 GPa

Piezoelectric co-efficient: d_{31}= -4.663 pC/N, d_{32}= -3.990 pC/N, d_{33}= 11.896 pC/N

$\mathbf{Li_{0.125}Ta_{0.125}Al_{0.750}N}$ (Li and Ta positions are swapped)

1.00000000000000

6.4995327069412312 0.0000000000000000 0.0000000000000000

-3.2497663534706156 5.6128725645051345 -0.0149727340141284

0.0000000000000000 -0.0264956911106536 9.7000418768101770

Al N Li Ta

12 16 2 2

Direct

0.1749376757239939 0.3337269801860612 0.0093180752408026

0.6587893044620604 0.3337269801860612 0.0093180752408026

0.1704697425111574 0.8409394850223221 -0.0008594247262572

0.6647978594862967 0.8295957189726001 0.9920247643115865

0.1639217884673883 0.8278435769347838 0.5075048508206028

0.6633899019022903 0.8267798038045880 0.5055477932557897

0.8349825987880644 0.1699651975761211 0.7517422160431994

0.3259543879039190 0.6663031354134951 0.7509484507135940

0.8403487475095831 0.6663031354134951 0.7509484507135940

0.8317453665638331 0.1634907331276587 0.2265651107717871

0.3335379815237529 0.6787615713408943 0.2347925567424577

0.8452235898171491 0.6787615713408943 0.2347925567424577

0.1601868620626578 0.3458024946657022 0.2119871993985639

0.6856156326030370 0.3458024946657022 0.2119871993985639

0.1590272988523816 0.8180545977047703 0.1908910624292174

0.6662418293410470 0.8324836586820999 0.1886508186355900

0.1505912288139538 0.3446630810626658 0.6738775224317873

0.6940718522487047 0.3446630810626658 0.6738775224317873

0.1567506953951406 0.8135013907902886 0.6948588091133653

0.6665083851868399 0.8330167703736864 0.6976907965555360

0.3360894827380689 0.1721789654761307 0.9614880577545988

0.8354910973641551 0.1709821947283033 0.9492906142934936

0.3322506083031074 0.6623247718741365 0.9456520816506930

0.8300741635710367 0.6623247718741365 0.9456520816506930

0.3223584350869114 0.1447168701738158 0.4469614944875228

0.8185557083925048 0.1371114167850024 0.4338167701025832

0.3463388169179623 0.6852772620668620 0.4395692892574846

0.8389384451489068 0.6852772620668620 0.4395692892574846

0.3307493263442491 0.1614986526884910 0.7525720447057803

0.3293662614531345 0.1587325229062621 0.2226293029161116

0.1669813440204601 0.3326949255167206 0.4731672838293708

0.6657135814962534 0.3326949255167206 0.4731672838293708

Elastic co-efficient: C_{11}= 310.98 GPa, C_{12}= 128.34 GPa, C_{33}= 178.53 GPa, C_{44}= 83.12 GPa

Piezoelectric co-efficient: d_{31}= -8.627 pC/N, d_{32}= -8.868 pC/N, d_{33}= 30.478 pC/N

$Li_{0.1875}Ta_{0.1875}Al_{0.6250}N$

1.00000000000000

6.5625183226627204 -0.0861316348642507 -0.0023919210640270

-3.3554691037723119 5.6873205153912387 -0.0059566959514051

-0.0030422698648814 -0.0132836149387547 9.7745088909349516

Al N Li Ta

10 16 3 3

Direct

0.1587511076295315 0.3169728518282852 0.0032647374960762

0.6725463308680215 0.3446243257844971 -0.0008511989617673

0.1533160438842261 0.8295883000948989 -0.0107966440542754

0.6654840126712056 0.3412653688364071 0.4914604557407056

0.1615780100282049 0.8302597528542195 0.5061920110989939

0.6645534297577357 0.8259451289904299 0.4845320637081523

0.3285448832091954 0.1577439876564481 0.7486792547022579

0.8365835273329567 0.6719392280750199 0.7506460754335668

0.3511949250958592 0.1699585029541825 0.2401048648939199

0.8329929664989039 0.6667310430859976 0.2438276604206437

0.1791781930088972 0.3229445162948765 0.2146872413785652

0.6671789959202139 0.3475900427711314 0.1905306673164471

0.1610200383735888 0.8519057883827157 0.1910590432087120

0.6779156917929751 0.8310278851585524 0.2184306975241950

0.1750611853764302 0.3173168553771549 0.6763986884897560

0.6557556250776110 0.3363887049568642 0.6873400167232542

0.1599762656692068 0.8410401026145315 0.6948110083772194

0.6787653447001633 0.8285175891702065 0.6833631742158154

0.3299976272734650 0.1671889418542633 0.9435796603458448

0.8450078877356200 0.1869709598267889 0.9330033748627652

0.3100145336478530 0.6504842242221587 0.9913368214266935

0.8377927043193143 0.6557090234978492 0.9384813010010535

0.3390115929680638 0.1558879187696341 0.4388489108661746

0.8177458469559165 0.1658338453887888 0.4649147351141049

0.3271411815871861 0.6774199222154184 0.4395980752709244

0.8351546758037593 0.6659435645873469 0.4421654328601018

0.6802616740696790 0.8316993444113328 -0.0061293868678816

0.3358465653467664 0.6706323184371686 0.7609890032383727

0.8218159702358155 0.1693160638322520 0.2376125908690402

0.1644664813722247 0.3311547860854476 0.4684498308991676

0.8318193536780206 0.1633362904245187 0.7332095394422360

0.3435273281113893 0.6766628215606137 0.2002602929591642

Elastic co-efficient: C_{11}= 274.29 GPa, C_{12}= 130.86 GPa, C_{33}= 162.05 GPa, C_{44}= 78.29 GPa

Piezoelectric co-efficient: d_{31}= -7.9128 pC/N, d_{32}= -8.973 pC/N, d_{33}= 27.620 pC/N

$Li_{0.1875}Ta_{0.1875}Al_{0.6250}N$ (Li and Ta positions are swapped)

1.00000000000000

6.6031094584972365 -0.0622595089490384 0.0059607521398315

-3.3558553457046649 5.6402416294595019 0.0023926599864097

0.0099878964674450 0.0092810223012890 9.7745571730818828

Al N Li Ta

10 16 3 3

Direct

0.1740550383196025 0.3354458881972676 -0.0154664959603834

0.6587334282357190 0.3345149600948884 -0.0085394567054169

0.1697412423132556 0.8384223215578150 0.0061923180808736

0.6553763528675715 0.3274524492765514 0.4991481558056040

0.1704081092180254 0.8466816154814553 0.4892054599621708

0.6830271238051021 0.8412479473594074 0.5032667788245090

0.3332725689167951 0.1670081693267629 0.7438291445164812

0.8300432417983646 0.6488049618587154 0.7401057653071806

0.3280613534558521 0.1634202886732502 0.2506457278801408

0.8422559509135362 0.6714550000159425 0.2486788186212018

0.1714821115584214 0.3212346575785070 0.1833626101361143

0.6636090063116008 0.3442426678924052 0.1873394546045018

0.1589594316792997 0.8400226220940525 0.1948101958284088

0.6826796358189327 0.8249365469969034 0.1763988812806356

0.1689681914132909 0.3220780907495129 0.7184305121771090

0.6524092594074234 0.3328186148753584 0.6905277981445311

0.1480958164916255 0.8389802333746531 0.6910602720464941

0.6770550305130328 0.8208221181154941 0.7146887851547075

0.3340592310202927 0.1648476218058593 0.9421657019219005

0.8341675905134885 0.1822555723283556 0.9649111587107009

0.3225781620768102 0.6728572730015898 0.9395976385119142

0.8441135219018191 0.6609888548782208 0.9388492871032919

0.3442910418962516 0.1622105893787989 0.4384797856522870

0.8130310088943428 0.1549942142579898 0.4330042434375070

0.3495149491556762 0.6899849691205110 0.4913361768947880

0.8328138119862182 0.6700043648712073 0.4435790342341291

0.1682991329345795 0.3197365902364210 0.4938706912280239

0.8306855407245827 0.1781826202750047 0.7376117661397390

0.3293642006967114 0.6641538602043598 0.2609907302421443

0.6688460614562686 0.8355351319852530 -0.0315509238688488

0.3233359708380341 0.6564740882068942 0.7002603336125525

0.8366668828674736 0.1681850959305919 0.2332096504750061

Elastic co-efficient: C_{11}= 279.63 GPa, C_{12}= 132.96 GPa, C_{33}= 160.80 GPa, C_{44}= 79.60 GPa

Piezoelectric co-efficient: d_{31}= -7.735 pC/N, d_{32}= -9.189 pC/N, d_{33}= 27.800 pC/N

$Sc_{0.125}Al_{0.875}N$ (configure#1)

1.00000000000000

6.3621913106733006 -0.0034811494430105 -0.0003756008033404

-3.1841104191847531 5.5150410229048603 0.0000000000000025

-0.0005973720574493 -0.0003448929181721 10.1180788447140575

Al N Sc

14 16 2

Direct

0.1646235910144571 0.3278157292345156 0.9957612039703558

0.6648831001594614 0.3324418000801031 0.9985287110696522

0.1646235910209088 0.8368083617793294 0.9957612039703985

0.6706145825436083 0.8353075412752849 0.9952712322437182

0.1656133426664961 0.3335570760637732 0.5010244005823129

0.6704388844742714 0.3352196922407091 0.4961009838852873

0.1656133426604351 0.8320567665958719 0.5010244005823342

0.3339419862742733 0.1669707431367749 0.7474159494345702

0.8327776276190680 0.1689782432511239 0.7522787151157428

0.3301640934930349 0.6650817967465396 0.7524458671609826

0.8327776276191107 0.6637988843684781 0.7522787151157073

0.3304756955215885 0.1652375977572777 0.2475177821675026

0.8361209355017482 0.1689216262399352 0.2444194821046453

0.8361209355026221 0.6671988092690686 0.2444194821046240

0.1574810831928824 0.3117292911307364 0.1824113445928785

0.6642876024165443 0.3321440512075929 0.1882782976534148

0.1574810832947458 0.8457522920629547 0.1824113445930490

0.6861091923647070 0.8430548462334694 0.1858479955540214

0.1646044379042008 0.3316612528735178 0.6920903476870824

0.6670956601208908 0.3335480800599510 0.6879926105309513

0.1646044379063822 0.8329436850317119 0.6920903476871180

0.6663241576778794 0.8331623288392375 0.7060861920139124

0.3349903526290597 0.1674949263151771 0.9361808281323856

0.8324803023503972 0.1691881376188037 0.9403176134451088

0.3307945570535664 0.6653970285261480 0.9446013688767491

0.8324803023475692 0.6632916647301098 0.9403176134450733

0.3331697302219202 0.1665846151114581 0.4404449367619205

0.8451835239660686 0.1872976689779262 0.4334607677982986

0.3176997870414638 0.6588496434710833 0.4477846357469689

0.8451835238644325 0.6578853549876961 0.4334607677981423

0.6723744864981105 0.8361874932491469 0.4999555953412363

0.3288664430780955 0.6644329715345080 0.2420192628338488

Elastic co-efficient: C_{11}= 333.85 GPa, C_{12}= 129.59 GPa, C_{33}= 296.07 GPa, C_{44}= 102.40 GPa

Piezoelectric co-efficient: d_{31}= -3.236 pC/N, d_{32}= -3.247 pC/N, d_{33}= 8.039 pC/N

$Sc_{0.125}Al_{0.875}N$(configure#2)

1.00000000000000

6.3682356153400672 -0.0000172503744209 -0.0000067726717169

-3.1841319999765596 5.5081452699044711 0.0003450261340014

-0.0000199976469191 0.0006305130129318 10.1180537662365637

Al N Sc

14 16 2

Direct

0.1721985621592781 0.3353874953228159 0.9957605086608520

0.6631891958443257 0.3353833618512471 0.9957622981161950

0.1675635735557617 0.8351186784253097 0.9985244170445549

0.6646976733568911 0.8293996261208456 0.9952751065660271

0.1664365452367823 0.3343926307638645 0.5010271795151675

0.6679587247245345 0.3343954452710027 0.5010260841413451

0.3310702692611461 0.6638716414055011 0.2444215916185722

0.1647933000983413 0.8295777177682006 0.4961096647750315

0.8349094821352071 0.1698240754248306 0.7524472943179163

0.3310228846344598 0.6672119319989822 0.7522691656457682

0.8361913426725244 0.6672152282374881 0.7522751900857623

0.3347492404220593 0.1695094067454859 0.2475209354077506

0.3330252766915995 0.1660490988296847 0.7474154070611199

0.8327968086775680 0.6638749764435006 0.2444218171118477

0.1882795171008003 0.3425188340076454 0.1824106098102674

0.6542389020278608 0.3425133728441571 0.1824162215771481

0.1678499728937637 0.8357067533123197 0.1882735137688472

0.6569414102281785 0.8138934112270065 0.1858545578057984

0.1683328309004697 0.3353833986590166 0.6920916239127020

0.6670560214425978 0.3353897245801605 0.6920951297963077

0.1664520411618538 0.8329020519089561 0.6879966407365025

0.6668402176300879 0.8336725245614223 0.7060751488440647

0.3325056555696098 0.1650077214674667 0.9361820487967896

0.8346079417514792 0.1692145417695194 0.9446060693483929

0.3308212218089949 0.6675249825318105 0.9403162217977351

0.8367063539670960 0.6675267585828578 0.9403208507446793

0.3334136622153209 0.1668367557075620 0.4404497517708569

0.8411454390830057 0.1822917220995807 0.4477784405617539

0.3126916495661173 0.6548158003876655 0.4334595530112644

0.8421244322988400 0.6548219801964338 0.4334612449678674

0.6638123971929206 0.8276187844939814 0.4999425006677736

0.8355774536905239 0.1711495670536779 0.2420132120133311

Elastic co-efficient: C_{11}= 336.26 GPa, C_{12}= 129.62 GPa, C_{33}= 295.77 GPa, C_{44}= 102.88 GPa

Piezoelectric co-efficient: d_{31}= -3.258 pC/N, d_{32}= -3.238 pC/N, d_{33}= 8.041 pC/N

$Sc_{0.25}Al_{0.75}N$(configure#1)

1.00000000000000

6.4590070624676974 0.0000000000000000 0.0000000000000000

-3.2295035312338487 5.6305502400753777 -0.0030804657599499

0.0000000000000000 -0.0055596390747375 10.1541078473220168

Al N Sc

12 16 4

Direct

0.1639312777058338 0.3396814572764642 0.0000632355746555

0.6757496795706245 0.3396814572764642 0.0000632355746555

0.1620516013603716 0.8241037027207420 -0.0000240377286877

0.6664701916747161 0.8329408833494384 0.9973309963411643

0.1654052438141743 0.8308109876283547 0.4961594353110511

0.6682091753070925 0.8364188506141907 0.4952243214558810

0.8324464313922562 0.1648923627845137 0.7544347374565186

0.3314631375344134 0.6649862239630088 0.7495169670888163

0.8335235864286011 0.6649862239630088 0.7495169670888163

0.8325741757187434 0.1651478514374811 0.2418103150259224

0.3347198139554159 0.6711500405088090 0.2452919886933050

0.8364307265533991 0.6711500405088090 0.2452919886933050

0.1574083504162850 0.3485841247686262 0.1885577277812119

0.6911752743523354 0.3485841247686262 0.1885577277812119

0.1542095492936344 0.8084195985872678 0.1843716922072562

0.6664606205307694 0.8329217410615444 0.1854341614484844

0.1568069645663080 0.3392677587432880 0.7011367791335902

0.6824602941769741 0.3392677587432880 0.7011367791335902

0.1544438859001257 0.8088882718002642 0.6860600761299082

0.6665667324979457 0.8331339649959043 0.6898855357160814

0.3329257696635048 0.1658510393269967 0.9642414283152507

0.8320750038153762 0.1641495076307535 0.9435990713024385

0.3352262806595785 0.6689779095321032 0.9392137813304593

0.8337521288725308 0.6689779095321032 0.9392137813304593

0.3242635209145384 0.1485265418290639 0.4425839418911063

0.8228739877631694 0.1457474755263334 0.4278418488373393

0.3457863279136271 0.6892838594535973 0.4336062173649580

0.8434980315399833 0.6892838594535973 0.4336062173649580

0.1641706021469536 0.3364953612759869 0.4942675386126194

0.6723242591290344 0.3364953612759869 0.4942675386126194

0.3292557086868138 0.1585109173736146 0.7542479677942600

0.3313416661448836 0.1626828322897687 0.2334900373367935

Elastic co-efficient: C_{11}= 309.45 GPa, C_{12}= 127.96 GPa, C_{33}= 247.63 GPa, C_{44}= 80.92 GPa

Piezoelectric co-efficient: d_{31}= -4.280 pC/N, d_{32}= -5.405 pC/N, d_{33}= 12.472 pC/N

$Sc_{0.25}Al_{0.75}N$(configure#2)

1.00000000000000

6.4475302299860822 0.0000000000000000 0.0000000000000000

-3.2237651149930411 5.5934645486943708 -0.0016127341735699

0.0000000000000000 -0.0027769950616594 10.2664899530349221

Al N Sc

12 16 4

Direct

0.1675585778043190 0.3359287888971961 0.0026000751589761

0.6683697110928710 0.3359287888971961 0.0026000751589761

0.1659908898032934 0.8319822796065854 0.0027013419974938

0.6662492372526474 0.8324989745053009 0.9970744721518532

0.1650227860618262 0.8300460721236582 0.4922848306195751

0.3314979828236326 0.1629954656472663 0.2419572047090810

0.8344262502053644 0.1688520004107301 0.7602046721679719

0.3283922774373200 0.6642219369075563 0.7548721131465077

0.8358301594702422 0.6642219369075563 0.7548721131465077

0.8328721590800308 0.1657438181600550 0.2374132426173080

0.3334461695936954 0.6704336101865163 0.2420187640610584

0.8369879405928263 0.6704336101865163 0.2420187640610584

0.1687894441250731 0.3362166028578373 0.1897882385200291

0.6674266587327583 0.3362166028578373 0.1897882385200291

0.1662927863672949 0.8325860727345888 0.1864672180148839

0.6658933614441341 0.8317872228882733 0.1849329238686835

0.1561531479439061 0.3400932999731185 0.6994589689748855

0.6839396520292065 0.3400932999731185 0.6994589689748855

0.1550197461756574 0.8100399923513274 0.6830292720610920

0.6668020645119123 0.8336046290238375 0.7073851042485720

0.3332026398263642 0.1664047796527155 0.9561554274609032

0.8341345857501932 0.1682686715003877 0.9479853749914651

0.3311945054468037 0.6674701896322230 0.9433246049885869

0.8362761841854249 0.6674701896322230 0.9433246049885869

0.3237178658786113 0.1474352317572094 0.4301814933435019

0.8319097299988906 0.1638189599977755 0.4199901359416282

0.3274521972890990 0.6790350975354986 0.4264043981103418

0.8515834002464129 0.6790350975354986 0.4264043981103418

0.1642088390034940 0.3356944525835073 0.4922842483970664

0.6714851135800147 0.3356944525835073 0.4922842483970664

0.3299992996094501 0.1599980992188874 0.7531549177311944

0.6678746366372437 0.8357497732744941 0.4975795453598885

Elastic co-efficient: C_{11}= 303.27 GPa, C_{12}= 121.44 GPa, C_{33}= 268.18 GPa, C_{44}= 90.15 GPa

Piezoelectric co-efficient: d_{31}= -3.803 pC/N, d_{32}= -3.862 pC/N, d_{33}= 9.173 pC/N

$Sc_{0.375}Al_{0.625}N$(configure#1)

1.00000000000000

6.6042765362350613 -0.0168243984668211 0.0019425459888895

-3.3167347355516981 5.7452996794500377 -0.0053435737634384

0.0033144229115681 -0.0080354083207553 10.1166297199617130

Al N Sc

10 16 6

Direct

0.1637459518166770 0.8375105614320653 0.0004674279619381

0.6719607651219150 0.8343073770603995 -0.0057246367386604

0.1703477675093670 0.3327409542780943 0.5038803656685629

0.6645018145115876 0.3393790766132250 0.5017646143960507

0.6688774689555405 0.8296352030381313 0.5014392777698183

0.3287760284395683 0.1598849953703844 0.7442731544878629

0.8325783766410741 0.1602448264436989 0.7400071968943465

0.8391029819002438 0.6767910992856717 0.7478075574846227

0.3369015406457150 0.1736612259037641 0.2505901905833258

0.8264838770328001 0.6640541262949624 0.2465535541856003

0.1728113570958574 0.3192846847831018 0.1915725552361339

0.6582805085996470 0.3412635300157349 0.1940413923892547

0.1571784082460561 0.8455813562743160 0.1967148369070997

0.6816794534035414 0.8266832521788274 0.1823300295067726

0.1612124494615430 0.3164289936473861 0.6956412176481401

0.6677986677941365 0.3377446802343712 0.6956032109040569

0.1564312159978031 0.8422758497595528 0.6907448669523348

0.6875253966977806 0.8402016470574085 0.6881046504652414

0.3231050618417153 0.1409629201349541 0.9306805136399785

0.8187570308095671 0.1424968972330510 0.9300522422216730

0.3398039071560056 0.6853438395210375 0.9542602038871679

0.8451728281866581 0.6881226370736129 0.9363308854010511

0.3451131044564908 0.1908595173402582 0.4410845407750519

0.8326114007540161 0.1680442610201992 0.4589392308453042

0.3423821543336720 0.6571762248740726 0.4545997313316207

0.8086541659087453 0.6552960402115574 0.4365332278758788

0.1637258891425563 0.3230405481758179 -0.0137617342366119

0.6653471419311857 0.3327267195554026 -0.0143806238008080

0.1621670854935041 0.8367463323689622 0.4870813675724169

0.3366278186243030 0.6736940235862503 0.7422269129804657

0.8321469535852094 0.1640595268801156 0.2505318310952112

0.3381914279055174 0.6637570723536130 0.2400102077090984

Elastic co-efficient: C_{11}= 278.79 GPa, C_{12}= 136.80 GPa, C_{33}= 178.54 GPa, C_{44}= 66.12 GPa

Piezoelectric co-efficient: d_{31}= -9.778 pC/N, d_{32}= -12.514 pC/N, d_{33}= 30.438 pC/N

$Sc_{0.375}Al_{0.625}N$(configure#2)

1.00000000000000

6.6042806885903289 -0.0229629632767150 0.0043747807590021

-3.3220774680557077 5.7511726920605888 -0.0080655888780580

0.0070955153954918 -0.0107186343140700 10.1178323797628575

Al N Sc

10 16 6

Direct

0.1670382592311981 0.8362957083715159 0.0012978779999244

0.6673197404589644 0.8320915585192807 0.9998552573797426

0.1781674721746143 0.3372734910268917 0.4967391761749624

0.6615203363993345 0.3429014115085067 0.5015646036394656

0.6644963220283273 0.8215461399106587 0.4958652483230850

0.3300881274010834 0.1627763469622607 0.7443058314205544

0.3373520484393069 0.6624562869773243 0.2475388684406994

0.8369439074748044 0.6747065450127394 0.7480011541538545

0.3384109844162353 0.1752990196717263 0.2508575954504195

0.8231332562942910 0.6608396859483392 0.2462809663443508

0.1802891867290697 0.3384757754526930 0.2018587671868488

0.6574168581109490 0.3402573294965094 0.1945804447190298

0.1664889768253772 0.8347837487563012 0.1993445988695655

0.6580604810851298 0.8140040084316951 0.1898445156523678

0.1842630312743410 0.3284161447510456 0.6865630587245377

0.6578650328484343 0.3490083350396915 0.6935997422558131

0.1565886454362868 0.8430873501051011 0.6890524623823566

0.6748799899991624 0.8163408472408449 0.6811791683377635

0.3211715965373116 0.1426060996555805 0.9326696798791687

0.8237425523410025 0.1449015387451240 0.9421006918034323

0.3409536092585057 0.6861114935110990 0.9506622019424142

0.8454303586424174 0.6905723880480465 0.9388476304863076

0.3458187746619643 0.1884664465592536 0.4387618885811904

0.8312667472335704 0.1679661755423822 0.4634331091471537

0.3436084073997208 0.6577715125157297 0.4397103161690694

0.8111278593336309 0.6547504391278025 0.4342425335277156

0.1692908427145241 0.3303517779347658 0.9952202284635234

0.6655354898203356 0.3341121831467859 0.9875358181712812

0.1642603146494608 0.8354187348359901 0.4838581226218821

0.3360781453420714 0.6718381406526603 0.7430704056657831

0.8281137372378282 0.1633487898268271 0.2520275853358243

0.8332789082007395 0.1612245467148341 0.7295304507499125

Elastic co-efficient: C_{11}= 276.89 GPa, C_{12}= 136.74 GPa, C_{33}= 184.08 GPa, C_{44}= 67.03 GPa

Piezoelectric co-efficient: d_{31}= -8.896 pC/N, d_{32}= -11.495 pC/N, d_{33}= 27.589 pC/N