

First Nanowire:

:POS001: ATOM -1 X,Y,Z = 0.50844 0.49156 0.96790 MULT= 1 ZZ= 49.000 In
:POS002: ATOM -2 X,Y,Z = 0.48307 0.51693 0.35875 MULT= 1 ZZ= 33.000 As
:POS003: ATOM -3 X,Y,Z = 0.68490 0.61931 0.85942 MULT= 1 ZZ= 33.000 As
:POS004: ATOM -4 X,Y,Z = 0.66051 0.56953 0.46755 MULT= 1 ZZ= 49.000 In
:POS005: ATOM -5 X,Y,Z = 0.73623 0.49385 0.96749 MULT= 1 ZZ= 49.000 In
:POS006: ATOM -6 X,Y,Z = 0.78597 0.51823 0.35946 MULT= 1 ZZ= 33.000 As
:POS007: ATOM -7 X,Y,Z = 0.68362 0.31638 0.85873 MULT= 1 ZZ= 33.000 As
:POS008: ATOM -8 X,Y,Z = 0.65817 0.34183 0.46807 MULT= 1 ZZ= 49.000 In
:POS009: ATOM -9 X,Y,Z = 0.50615 0.26377 0.96749 MULT= 1 ZZ= 49.000 In
:POS010: ATOM -10 X,Y,Z = 0.48177 0.21403 0.35946 MULT= 1 ZZ= 33.000 As
:POS011: ATOM -11 X,Y,Z = 0.38069 0.31510 0.85942 MULT= 1 ZZ= 33.000 As
:POS012: ATOM -12 X,Y,Z = 0.43047 0.33949 0.46755 MULT= 1 ZZ= 49.000 In

TOTAL ENERGY IN Ry = -97780.50383992

Second Nanowire

:POS001: ATOM -1 X,Y,Z = 0.29682 0.24040 0.89523 MULT= 1 ZZ= 33.000 As
:POS002: ATOM -2 X,Y,Z = 0.34102 0.25666 0.51344 MULT= 1 ZZ= 49.000 In
:POS003: ATOM -3 X,Y,Z = 0.40732 0.21574 0.99565 MULT= 1 ZZ= 49.000 In
:POS004: ATOM -4 X,Y,Z = 0.37955 0.15996 0.37746 MULT= 1 ZZ= 33.000 As
:POS005: ATOM -5 X,Y,Z = 0.54296 0.24155 0.89577 MULT= 1 ZZ= 33.000 As
:POS006: ATOM -6 X,Y,Z = 0.51487 0.25701 0.51372 MULT= 1 ZZ= 49.000 In
:POS007: ATOM -7 X,Y,Z = 0.60851 0.39149 0.94888 MULT= 1 ZZ= 49.000 In
:POS008: ATOM -8 X,Y,Z = 0.60578 0.39422 0.36140 MULT= 1 ZZ= 33.000 As
:POS009: ATOM -9 X,Y,Z = 0.75845 0.45704 0.89577 MULT= 1 ZZ= 33.000 As

:POS010: ATOM -10 X,Y,Z = 0.74299 0.48513 0.51372 MULT= 1 ZZ= 49.000 In
:POS011: ATOM -11 X,Y,Z = 0.78426 0.59268 0.99566 MULT= 1 ZZ= 49.000 In
:POS012: ATOM -12 X,Y,Z = 0.84004 0.62045 0.37746 MULT= 1 ZZ= 33.000 As
:POS013: ATOM -13 X,Y,Z = 0.75960 0.70318 0.89524 MULT= 1 ZZ= 33.000 As
:POS014: ATOM -14 X,Y,Z = 0.74334 0.65898 0.51344 MULT= 1 ZZ= 49.000 In
:POS015: ATOM -15 X,Y,Z = 0.60951 0.61865 0.94876 MULT= 1 ZZ= 49.000 In
:POS016: ATOM -16 X,Y,Z = 0.60589 0.61077 0.36117 MULT= 1 ZZ= 33.000 As
:POS017: ATOM -17 X,Y,Z = 0.54377 0.70267 0.89534 MULT= 1 ZZ= 33.000 As
:POS018: ATOM -18 X,Y,Z = 0.51663 0.65878 0.51287 MULT= 1 ZZ= 49.000 In
:POS019: ATOM -19 X,Y,Z = 0.40818 0.59182 0.99620 MULT= 1 ZZ= 49.000 In
:POS020: ATOM -20 X,Y,Z = 0.38077 0.61923 0.37877 MULT= 1 ZZ= 33.000 As
:POS021: ATOM -21 X,Y,Z = 0.29733 0.45623 0.89534 MULT= 1 ZZ= 33.000 As
:POS022: ATOM -22 X,Y,Z = 0.34122 0.48337 0.51287 MULT= 1 ZZ= 49.000 In
:POS023: ATOM -23 X,Y,Z = 0.38135 0.39049 0.94876 MULT= 1 ZZ= 49.000 In
:POS024: ATOM -24 X,Y,Z = 0.38923 0.39411 0.36117 MULT= 1 ZZ= 33.000 As
:POS025: ATOM -25 X,Y,Z = 0.53307 0.46693 0.86994 MULT= 1 ZZ= 33.000 As
:POS026: ATOM -26 X,Y,Z = 0.53372 0.46628 0.46351 MULT= 1 ZZ= 49.000 In
TOTAL ENERGY IN Ry = -211858.59304237

Third Nanowire

:POS001: ATOM -1 X,Y,Z = 0.69134 0.79912 0.89182 MULT= 1 ZZ= 33.000 As
:POS002: ATOM -2 X,Y,Z = 0.67796 0.76174 0.52111 MULT= 1 ZZ= 49.000 In
:POS003: ATOM -3 X,Y,Z = 0.71420 0.72557 0.02111 MULT= 1 ZZ= 49.000 In
:POS004: ATOM -4 X,Y,Z = 0.75157 0.73897 0.39183 MULT= 1 ZZ= 33.000 As
:POS005: ATOM -5 X,Y,Z = 0.68194 0.62712 0.86865 MULT= 1 ZZ= 33.000 As

:POS006: ATOM -6 X,Y,Z = 0.69223 0.63227 0.46413 MULT= 1 ZZ= 49.000 In
:POS007: ATOM -7 X,Y,Z = 0.71363 0.56061 0.02103 MULT= 1 ZZ= 49.000 In
:POS008: ATOM -8 X,Y,Z = 0.75124 0.58459 0.39180 MULT= 1 ZZ= 33.000 As
:POS009: ATOM -9 X,Y,Z = 0.69077 0.46416 0.89154 MULT= 1 ZZ= 33.000 As
:POS010: ATOM -10 X,Y,Z = 0.67736 0.48788 0.52032 MULT= 1 ZZ= 49.000 In
:POS011: ATOM -11 X,Y,Z = 0.58406 0.41595 0.96353 MULT= 1 ZZ= 49.000 In
:POS012: ATOM -12 X,Y,Z = 0.57899 0.42100 0.36791 MULT= 1 ZZ= 33.000 As
:POS013: ATOM -13 X,Y,Z = 0.53596 0.30925 0.89155 MULT= 1 ZZ= 33.000 As
:POS014: ATOM -14 X,Y,Z = 0.51220 0.32261 0.52032 MULT= 1 ZZ= 49.000 In
:POS015: ATOM -15 X,Y,Z = 0.43947 0.28627 0.02105 MULT= 1 ZZ= 49.000 In
:POS016: ATOM -16 X,Y,Z = 0.41552 0.24866 0.39181 MULT= 1 ZZ= 33.000 As
:POS017: ATOM -17 X,Y,Z = 0.37288 0.31786 0.86867 MULT= 1 ZZ= 33.000 As
:POS018: ATOM -18 X,Y,Z = 0.36773 0.30758 0.46414 MULT= 1 ZZ= 49.000 In
:POS019: ATOM -19 X,Y,Z = 0.27441 0.28552 0.02113 MULT= 1 ZZ= 49.000 In
:POS020: ATOM -20 X,Y,Z = 0.26104 0.24815 0.39186 MULT= 1 ZZ= 33.000 As
:POS021: ATOM -21 X,Y,Z = 0.20080 0.30829 0.89185 MULT= 1 ZZ= 33.000 As
:POS022: ATOM -22 X,Y,Z = 0.23818 0.32170 0.52113 MULT= 1 ZZ= 49.000 In
:POS023: ATOM -23 X,Y,Z = 0.26015 0.41500 0.96413 MULT= 1 ZZ= 49.000 In
:POS024: ATOM -24 X,Y,Z = 0.27044 0.42015 0.36866 MULT= 1 ZZ= 33.000 As
:POS025: ATOM -25 X,Y,Z = 0.20115 0.46269 0.89180 MULT= 1 ZZ= 33.000 As
:POS026: ATOM -26 X,Y,Z = 0.23875 0.48666 0.52103 MULT= 1 ZZ= 49.000 In
:POS027: ATOM -27 X,Y,Z = 0.27503 0.55939 0.02031 MULT= 1 ZZ= 49.000 In
:POS028: ATOM -28 X,Y,Z = 0.26162 0.58312 0.39152 MULT= 1 ZZ= 33.000 As
:POS029: ATOM -29 X,Y,Z = 0.37340 0.62625 0.86789 MULT= 1 ZZ= 33.000 As
:POS030: ATOM -30 X,Y,Z = 0.36833 0.63131 0.46353 MULT= 1 ZZ= 49.000 In

:POS031: ATOM -31 X,Y,Z = 0.44019 0.72464 0.02029 MULT= 1 ZZ= 49.000 In
:POS032: ATOM -32 X,Y,Z = 0.41643 0.73801 0.39151 MULT= 1 ZZ= 33.000 As
:POS033: ATOM -33 X,Y,Z = 0.53686 0.79860 0.89177 MULT= 1 ZZ= 33.000 As
:POS034: ATOM -34 X,Y,Z = 0.51291 0.76098 0.52102 MULT= 1 ZZ= 49.000 In
:POS035: ATOM -35 X,Y,Z = 0.58465 0.73969 0.96413 MULT= 1 ZZ= 49.000 In
:POS036: ATOM -36 X,Y,Z = 0.57949 0.72937 0.36864 MULT= 1 ZZ= 33.000 As
:POS037: ATOM -37 X,Y,Z = 0.52996 0.63092 0.87272 MULT= 1 ZZ= 33.000 As
:POS038: ATOM -38 X,Y,Z = 0.52667 0.62489 0.47332 MULT= 1 ZZ= 49.000 In
:POS039: ATOM -39 X,Y,Z = 0.57746 0.57420 0.97332 MULT= 1 ZZ= 49.000 In
:POS040: ATOM -40 X,Y,Z = 0.58347 0.57748 0.37273 MULT= 1 ZZ= 33.000 As
:POS041: ATOM -41 X,Y,Z = 0.52983 0.47008 0.87213 MULT= 1 ZZ= 33.000 As
:POS042: ATOM -42 X,Y,Z = 0.52675 0.47315 0.47269 MULT= 1 ZZ= 49.000 In
:POS043: ATOM -43 X,Y,Z = 0.42571 0.42234 0.97332 MULT= 1 ZZ= 49.000 In
:POS044: ATOM -44 X,Y,Z = 0.42242 0.41633 0.37273 MULT= 1 ZZ= 33.000 As
:POS045: ATOM -45 X,Y,Z = 0.36891 0.46976 0.87273 MULT= 1 ZZ= 33.000 As
:POS046: ATOM -46 X,Y,Z = 0.37492 0.47305 0.47332 MULT= 1 ZZ= 49.000 In
:POS047: ATOM -47 X,Y,Z = 0.42564 0.57410 0.97269 MULT= 1 ZZ= 49.000 In
:POS048: ATOM -48 X,Y,Z = 0.42254 0.57718 0.37213 MULT= 1 ZZ= 33.000 As
TOTAL ENERGY IN Ry = -391121.24277224

Fourth Nanowire

:POS001: ATOM -1 POSITION = 0.44004 0.14990 0.03045 MULTIPLICITY = 1 ZZ= 49.000 In
:POS002: ATOM -2 POSITION = 0.41501 0.11202 0.39686 MULTIPLICITY = 1 ZZ= 33.000 As
:POS003: ATOM -3 POSITION = 0.53202 0.17076 0.89315 MULTIPLICITY = 1 ZZ= 33.000 As
:POS004: ATOM -4 POSITION = 0.50989 0.18474 0.53030 MULTIPLICITY = 1 ZZ= 49.000 In

:POS005: ATOM -5 POSITION = 0.57964 0.27516 0.97164 MULTIPLICITY = 1 ZZ= 49.000 In
:POS006: ATOM -6 POSITION = 0.57227 0.27722 0.36457 MULTIPLICITY = 1 ZZ= 33.000 As
:POS007: ATOM -7 POSITION = 0.68306 0.31690 0.90277 MULTIPLICITY = 1 ZZ= 33.000 As
:POS008: ATOM -8 POSITION = 0.66523 0.33474 0.54202 MULTIPLICITY = 1 ZZ= 49.000 In
:POS009: ATOM -9 POSITION = 0.72481 0.42032 0.97164 MULTIPLICITY = 1 ZZ= 49.000 In
:POS010: ATOM -10 POSITION = 0.72275 0.42769 0.36458 MULTIPLICITY = 1 ZZ= 33.000 As
:POS011: ATOM -11 POSITION = 0.82920 0.46793 0.89315 MULTIPLICITY = 1 ZZ= 33.000 As
:POS012: ATOM -12 POSITION = 0.81524 0.49007 0.53031 MULTIPLICITY = 1 ZZ= 49.000 In
:POS013: ATOM -13 POSITION = 0.85007 0.55992 0.03044 MULTIPLICITY = 1 ZZ= 49.000 In
:POS014: ATOM -14 POSITION = 0.88795 0.58494 0.39685 MULTIPLICITY = 1 ZZ= 33.000 As
:POS015: ATOM -15 POSITION = 0.82228 0.62628 0.87038 MULTIPLICITY = 1 ZZ= 33.000 As
:POS016: ATOM -16 POSITION = 0.82865 0.62869 0.47589 MULTIPLICITY = 1 ZZ= 49.000 In
:POS017: ATOM -17 POSITION = 0.84986 0.72053 0.02997 MULTIPLICITY = 1 ZZ= 49.000 In
:POS018: ATOM -18 POSITION = 0.88752 0.73164 0.39114 MULTIPLICITY = 1 ZZ= 33.000 As
:POS019: ATOM -19 POSITION = 0.82753 0.79133 0.89488 MULTIPLICITY = 1 ZZ= 33.000 As
:POS020: ATOM -20 POSITION = 0.81900 0.75604 0.53185 MULTIPLICITY = 1 ZZ= 49.000 In
:POS021: ATOM -21 POSITION = 0.72392 0.73429 0.97422 MULTIPLICITY = 1 ZZ= 49.000 In
:POS022: ATOM -22 POSITION = 0.72426 0.72642 0.36719 MULTIPLICITY = 1 ZZ= 33.000 As
:POS023: ATOM -23 POSITION = 0.68294 0.79587 0.90557 MULTIPLICITY = 1 ZZ= 33.000 As
:POS024: ATOM -24 POSITION = 0.66726 0.76180 0.54257 MULTIPLICITY = 1 ZZ= 49.000 In
:POS025: ATOM -25 POSITION = 0.58100 0.73300 0.97438 MULTIPLICITY = 1 ZZ= 49.000 In
:POS026: ATOM -26 POSITION = 0.57377 0.72455 0.36757 MULTIPLICITY = 1 ZZ= 33.000 As
:POS027: ATOM -27 POSITION = 0.53319 0.78861 0.89616 MULTIPLICITY = 1 ZZ= 33.000 As
:POS028: ATOM -28 POSITION = 0.50963 0.75461 0.53015 MULTIPLICITY = 1 ZZ= 49.000 In
:POS029: ATOM -29 POSITION = 0.44128 0.71879 0.03023 MULTIPLICITY = 1 ZZ= 49.000 In

:POS030: ATOM -30 POSITION = 0.41681 0.73154 0.39159 MULTIPLICITY = 1 ZZ= 33.000 As
:POS031: ATOM -31 POSITION = 0.37611 0.62390 0.86757 MULTIPLICITY = 1 ZZ= 33.000 As
:POS032: ATOM -32 POSITION = 0.37183 0.62818 0.47153 MULTIPLICITY = 1 ZZ= 49.000 In
:POS033: ATOM -33 POSITION = 0.28122 0.55874 0.03024 MULTIPLICITY = 1 ZZ= 49.000 In
:POS034: ATOM -34 POSITION = 0.26847 0.58321 0.39159 MULTIPLICITY = 1 ZZ= 33.000 As
:POS035: ATOM -35 POSITION = 0.21139 0.46683 0.89616 MULTIPLICITY = 1 ZZ= 33.000 As
:POS036: ATOM -36 POSITION = 0.24539 0.49039 0.53016 MULTIPLICITY = 1 ZZ= 49.000 In
:POS037: ATOM -37 POSITION = 0.26699 0.41902 0.97438 MULTIPLICITY = 1 ZZ= 49.000 In
:POS038: ATOM -38 POSITION = 0.27544 0.42624 0.36757 MULTIPLICITY = 1 ZZ= 33.000 As
:POS039: ATOM -39 POSITION = 0.20411 0.31707 0.90558 MULTIPLICITY = 1 ZZ= 33.000 As
:POS040: ATOM -40 POSITION = 0.23818 0.33275 0.54257 MULTIPLICITY = 1 ZZ= 49.000 In
:POS041: ATOM -41 POSITION = 0.26569 0.27609 0.97423 MULTIPLICITY = 1 ZZ= 49.000 In
:POS042: ATOM -42 POSITION = 0.27355 0.27574 0.36719 MULTIPLICITY = 1 ZZ= 33.000 As
:POS043: ATOM -43 POSITION = 0.20864 0.17247 0.89489 MULTIPLICITY = 1 ZZ= 33.000 As
:POS044: ATOM -44 POSITION = 0.24393 0.18100 0.53185 MULTIPLICITY = 1 ZZ= 49.000 In
:POS045: ATOM -45 POSITION = 0.27943 0.15013 0.02997 MULTIPLICITY = 1 ZZ= 49.000 In
:POS046: ATOM -46 POSITION = 0.26832 0.11248 0.39114 MULTIPLICITY = 1 ZZ= 33.000 As
:POS047: ATOM -47 POSITION = 0.37368 0.17771 0.87037 MULTIPLICITY = 1 ZZ= 33.000 As
:POS048: ATOM -48 POSITION = 0.37127 0.17134 0.47590 MULTIPLICITY = 1 ZZ= 49.000 In
:POS049: ATOM -49 POSITION = 0.42578 0.27985 0.97329 MULTIPLICITY = 1 ZZ= 49.000 In
:POS050: ATOM -50 POSITION = 0.42122 0.27367 0.36943 MULTIPLICITY = 1 ZZ= 33.000 As
:POS051: ATOM -51 POSITION = 0.52556 0.32484 0.87019 MULTIPLICITY = 1 ZZ= 33.000 As
:POS052: ATOM -52 POSITION = 0.52313 0.32862 0.47625 MULTIPLICITY = 1 ZZ= 49.000 In
:POS053: ATOM -53 POSITION = 0.57422 0.42576 0.97212 MULTIPLICITY = 1 ZZ= 49.000 In
:POS054: ATOM -54 POSITION = 0.57341 0.42657 0.36327 MULTIPLICITY = 1 ZZ= 33.000 As

:POS055: ATOM -55 POSITION = 0.67514 0.47441 0.87019 MULTIPLICITY = 1 ZZ= 33.000 As
:POS056: ATOM -56 POSITION = 0.67136 0.47684 0.47625 MULTIPLICITY = 1 ZZ= 49.000 In
:POS057: ATOM -57 POSITION = 0.72014 0.57419 0.97329 MULTIPLICITY = 1 ZZ= 49.000 In
:POS058: ATOM -58 POSITION = 0.72631 0.57875 0.36943 MULTIPLICITY = 1 ZZ= 33.000 As
:POS059: ATOM -59 POSITION = 0.67667 0.63156 0.87038 MULTIPLICITY = 1 ZZ= 33.000 As
:POS060: ATOM -60 POSITION = 0.67384 0.62608 0.47622 MULTIPLICITY = 1 ZZ= 49.000 In
:POS061: ATOM -61 POSITION = 0.57389 0.57566 0.97214 MULTIPLICITY = 1 ZZ= 49.000 In
:POS062: ATOM -62 POSITION = 0.57391 0.57524 0.36415 MULTIPLICITY = 1 ZZ= 33.000 As
:POS063: ATOM -63 POSITION = 0.52674 0.62875 0.87034 MULTIPLICITY = 1 ZZ= 33.000 As
:POS064: ATOM -64 POSITION = 0.52412 0.62459 0.47620 MULTIPLICITY = 1 ZZ= 49.000 In
:POS065: ATOM -65 POSITION = 0.42621 0.57379 0.97404 MULTIPLICITY = 1 ZZ= 49.000 In
:POS066: ATOM -66 POSITION = 0.42345 0.57655 0.36925 MULTIPLICITY = 1 ZZ= 33.000 As
:POS067: ATOM -67 POSITION = 0.37124 0.47326 0.87034 MULTIPLICITY = 1 ZZ= 33.000 As
:POS068: ATOM -68 POSITION = 0.37539 0.47588 0.47620 MULTIPLICITY = 1 ZZ= 49.000 In
:POS069: ATOM -69 POSITION = 0.42432 0.42610 0.97215 MULTIPLICITY = 1 ZZ= 49.000 In
:POS070: ATOM -70 POSITION = 0.42474 0.42607 0.36414 MULTIPLICITY = 1 ZZ= 33.000 As
:POS071: ATOM -71 POSITION = 0.36841 0.32332 0.87038 MULTIPLICITY = 1 ZZ= 33.000 As
:POS072: ATOM -72 POSITION = 0.37390 0.32616 0.47623 MULTIPLICITY = 1 ZZ= 49.000 In
:POS073: ATOM -73 POSITION = 0.52382 0.47616 0.86506 MULTIPLICITY = 1 ZZ= 33.000 As
:POS074: ATOM -74 POSITION = 0.52389 0.47610 0.47970 MULTIPLICITY = 1 ZZ= 49.000 In
TOTAL ENERGY IN Ry = -602963.30828942
