:KPT : NUMBER OF K-POINTS: 2

Insulator, EF-inconsistency corrected

:GAP : 0.2386 Ry = 3.244 eV (provided you have a proper k-mesh)

Bandranges (emin - emax) and occupancy:

:BAN00238: 238 0.174430 0.174688 1.00000000

:BAN00239: 239 0.176158 0.178048 1.00000000

:BAN00240: 240 0.178923 0.181436 1.00000000

:BAN00241: 241 0.182661 0.185641 1.00000000

:BAN00242: 242 0.185706 0.186223 1.00000000

:BAN00243: 243 0.188023 0.189149 1.00000000

:BAN00244: 244 0.189908 0.191509 1.00000000

:BAN00245: 245 0.194415 0.194773 1.00000000

:BAN00246: 246 0.194827 0.196938 1.00000000

:BAN00247: 247 0.197742 0.198420 1.00000000

:BAN00248: 248 0.199951 0.200536 1.00000000

:BAN00249: 249 0.439091 0.440245 0.00000000

:BAN00250: 250 0.446376 0.448097 0.00000000

:BAN00251: 251 0.447746 0.448749 0.00000000

:BAN00252: 252 0.448622 0.451047 0.00000000

:BAN00253: 253 0.451482 0.453211 0.00000000

Energy to separate low and high energystates: -0.27459

:NOE : NUMBER OF ELECTRONS = 496.000

:FER : F E R M I - ENERGY(TETRAH.M.)= 0.2005356426

:GMA : POTENTIAL AND CHARGE CUT-OFF 12.00 Ry\*\*.5

:POS001: ATOM -1 X,Y,Z = 0.37457 0.77849 0.69116 MULT= 4 ZZ= 19.000

Insulator, EF-inconsistency corrected

:GAP : 0.2385 Ry = 3.244 eV (provided you have a proper k-mesh)

Bandranges (emin - emax) and occupancy:

:BAN00238: 238 0.174420 0.174699 1.00000000

:BAN00239: 239 0.176159 0.178032 1.00000000

:BAN00240: 240 0.178903 0.181440 1.00000000

:BAN00241: 241 0.182643 0.185619 1.00000000

:BAN00242: 242 0.185732 0.186245 1.00000000

:BAN00243: 243 0.187994 0.189150 1.00000000

:BAN00244: 244 0.189888 0.191465 1.00000000

:BAN00245: 245 0.194360 0.194722 1.00000000

:BAN00246: 246 0.194797 0.196890 1.00000000

:BAN00247: 247 0.197707 0.198381 1.00000000

:BAN00248: 248 0.199907 0.200521 1.00000000

:BAN00249: 249 0.439036 0.440186 0.00000000

:BAN00250: 250 0.446706 0.448161 0.00000000

:BAN00251: 251 0.447901 0.449004 0.00000000

:BAN00252: 252 0.448963 0.451300 0.00000000

:BAN00253: 253 0.451907 0.453485 0.00000000

Energy to separate low and high energystates: -0.27458

:NOE : NUMBER OF ELECTRONS = 496.000

:FER : F E R M I - ENERGY(TETRAH.M.)= 0.2005356426

:GMA : POTENTIAL AND CHARGE CUT-OFF 12.00 Ry\*\*.5

:POS001: ATOM -1 X,Y,Z = 0.37457 0.77849 0.69116 MULT= 4 ZZ= 19.000

K

LMMAX 49

:

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0.49506

:GAP : -99999. Ry = -9999. eV ( metallic )

Bandranges (emin - emax) and occupancy:

:BAN00038: 38 -2.152824 -2.152812 1.00000000

:BAN00039: 39 -2.152774 -2.152752 1.00000000

:BAN00040: 40 -2.152708 -2.152705 1.00000000

:BAN00041: 41 -2.151804 -2.151802 1.00000000

:BAN00042: 42 -2.151671 -2.151669 1.00000000

:BAN00043: 43 -2.151446 -2.151443 1.00000000

:BAN00044: 44 -2.151298 -2.151264 1.00000000

:BAN00045: 45 -2.136739 -2.136736 1.00000000

:BAN00046: 46 -2.136544 -2.136515 1.00000000

:BAN00047: 47 -2.136211 -2.136162 1.00000000

:BAN00048: 48 -2.135804 -2.135786 1.00000000

:BAN00049: 49 -2.135045 -2.134929 0.00000000

:BAN00050: 50 -2.134989 -2.134904 0.00000000

:BAN00051: 51 -2.134934 -2.134880 0.00000000

:BAN00052: 52 -2.134925 -2.134867 0.00000000

:BAN00053: 53 -2.133068 -2.133067 0.00000000

Energy to separate low and high energystates: -2.20588

:NOE : NUMBER OF ELECTRONS = 96.000

:FER : F E R M I - ENERGY(TETRAH.M.)= -2.1355977921

:GMA : POTENTIAL AND CHARGE CUT-OFF 12.00 Ry\*\*.5

:POS001: ATOM -1 X,Y,Z = 0.37457 0.77849 0.69116 MULT= 4 ZZ= 19.000

K

LMMAX 49