Fermi Energy in Density of States Calculation for LaPO4

|  |  |  |  |
| --- | --- | --- | --- |
| K-point | EFermi (SCF) | EFermi (SCF) | EFermi (DOS) used in plotting the graph |
| 10 | 12.8279 | 7.1779 | 7.1779 |
| 12 | 12.8279 | 12.9084 | 7.1779 |
| 14 | 12.8279 | 12.9084 | 7.1779 |
| 16 | 12.8279 | 7.1779 | 7.1779 |
| 18 | 12.8279 | 7.1778 | 7.1779 |



SCF Input

&control

 calculation = 'scf'

 restart\_mode='from\_scratch',

 prefix='LaPO4',

 pseudo\_dir ='/home2/yogesh/Mywork/PhD/LaPO4/Pure/pbepaw/',

 outdir='/home2/yogesh/Mywork/PhD/LaPO4/Pure/pbepaw/ambient/dos/outdir',

 /

 &SYSTEM

 ibrav= 0,

 celldm(1) = 13.0,

 nat = 24,

 ntyp = 3,

 ecutwfc = 80 ,

 ecutrho = 400 ,

 occupations = 'smearing' ,

 degauss = 0.05 ,

 smearing = 'methfessel-paxton' ,

 /

 &ELECTRONS

 conv\_thr = 1D-8 ,

 mixing\_mode = 'TF' ,

 mixing\_beta = 0.7 ,

 /

CELL\_PARAMETERS alat

 1.0063000 0.000000000 0.001154019

 0.000000000 1.037206297 0.000000000

 -0.224024481 0.000000000 0.924622174

ATOMIC\_SPECIES

 La 138.90000 La.pbe-n-bpaw.UPF

 P 30.97300 P.pbe-n-kjpaw\_psl.0.1.upf

 O 15.99900 O.pbe-n-kjpaw\_psl.0.1.upf

ATOMIC\_POSITIONS crystal

La 0.284590303 0.157248128 0.097447480

La 0.715409727 0.842751858 0.902552497

La 0.215409697 0.657248142 0.402552527

La 0.784590273 0.342751858 0.597447503

P 0.303366323 0.161549460 0.611278232

P 0.696633647 0.838450525 0.388721768

P 0.196633677 0.661549475 0.888721768

P 0.803366353 0.338450525 0.111278232

O 0.250071384 0.006421307 0.441770872

O 0.749928616 0.993578667 0.558229098

O 0.249928616 0.506421333 0.058229128

O 0.750071384 0.493578697 0.941770902

O 0.381031881 0.329917127 0.499694968

O 0.618968148 0.670082873 0.500305032

O 0.118968119 0.829917127 0.000305032

O 0.881031852 0.170082873 0.999694968

O 0.469674074 0.103432586 0.804875915

O 0.530325926 0.896567406 0.195124085

O 0.030325926 0.603432594 0.695124085

O 0.969674074 0.396567406 0.304875915

O 0.126892375 0.211812137 0.708352777

O 0.873107655 0.788187893 0.291647223

O 0.373107625 0.711812107 0.791647223

O 0.626892345 0.288187863 0.208352777

K\_POINTS automatic

 10 10 10 0 0 0

NSCF Input

&control

 calculation = 'nscf'

 restart\_mode='from\_scratch',

 prefix='LaPO4',

 pseudo\_dir ='/home2/yogesh/Mywork/PhD/LaPO4/Pure/pbpaw/',

 outdir='/home2/yogesh/Mywork/PhD/LaPO4/Pure/pbepaw/ambient/dos/outdir/',

 /

 &SYSTEM

 ibrav= 0,

 celldm(1) = 13.0,

 nat = 24,

 ntyp = 3,

 ecutwfc = 80 ,

 ecutrho = 400 ,

 occupations = 'tetrahedra' ,

 degauss = 0.05 ,

 smearing = 'methfessel-paxton' ,

 /

 &ELECTRONS

 conv\_thr = 1D-8 ,

 mixing\_mode = 'TF' ,

 mixing\_beta = 0.7 ,

 /

CELL\_PARAMETERS alat

 1.0063000 0.000000000 0.001154019

 0.000000000 1.037206297 0.000000000

 -0.224024481 0.000000000 0.924622174

ATOMIC\_SPECIES

 La 138.90000 La.pbe-n-bpaw.UPF

 P 30.97300 P.pbe-n-kjpaw\_psl.0.1.upf

 O 15.99900 O.pbe-n-kjpaw\_psl.0.1.upf

ATOMIC\_POSITIONS crystal

La 0.284590303 0.157248128 0.097447480

La 0.715409727 0.842751858 0.902552497

La 0.215409697 0.657248142 0.402552527

La 0.784590273 0.342751858 0.597447503

P 0.303366323 0.161549460 0.611278232

P 0.696633647 0.838450525 0.388721768

P 0.196633677 0.661549475 0.888721768

P 0.803366353 0.338450525 0.111278232

O 0.250071384 0.006421307 0.441770872

O 0.749928616 0.993578667 0.558229098

O 0.249928616 0.506421333 0.058229128

O 0.750071384 0.493578697 0.941770902

O 0.381031881 0.329917127 0.499694968

O 0.618968148 0.670082873 0.500305032

O 0.118968119 0.829917127 0.000305032

O 0.881031852 0.170082873 0.999694968

O 0.469674074 0.103432586 0.804875915

O 0.530325926 0.896567406 0.195124085

O 0.030325926 0.603432594 0.695124085

O 0.969674074 0.396567406 0.304875915

O 0.126892375 0.211812137 0.708352777

O 0.873107655 0.788187893 0.291647223

O 0.373107625 0.711812107 0.791647223

O 0.626892345 0.288187863 0.208352777

K\_POINTS automatic

 10 10 10 0 0 0

DOS Input

&DOS

 prefix = 'LaPO4' ,

 outdir = '/home2/yogesh/Mywork/PhD/LaPO4/Pure/pbepaw/ambient/dos/outdir/' ,

 fildos = 'LaPO4.dos-0.01.dat' ,

 DeltaE = 0.01 ,

 /