

ftn58sparse =

struct with fields:

System: 'Bi2Se3\_bulk' → the name of the system  
Ainfo: [1x5 struct] → information about atoms  
  abc: [9.8390 9.8390 9.8390] → lattice constants  
  BR: [3x3 double] → Bravais vectors  
  Nat: 5 → # of atoms  
  ver: 'type1' → { type 1: Bloch basis  
                  type 2: Wannier basis  
isSO: 1 → Whether both spins are considered or not  
  norb: 40 → # of spin-orbitals  
Orbitps: [40x7 double] → information about spin-orbitals  
  ij: [2980x2 double]  
  tt: [2980x1 double]  
  dd: [2980x3 double]

```
ftn58sparse.abc
```

```
ans =
```

```
9.8390    9.8390    9.8390
```

```
ftn58sparse.BR
```

```
ans =
```

```
-0.2091    -0.1207    0.9704  
 0.2091    -0.1207    0.9704  
      0      0.2414    0.9704
```

$$\begin{cases} \vec{a} = a \cdot ( \text{BR}(\textcolor{red}{1},\textcolor{blue}{1})\hat{x} + \text{BR}(\textcolor{red}{1},\textcolor{blue}{2})\hat{y} + \text{BR}(\textcolor{red}{1},\textcolor{blue}{3})\hat{z} ) \\ \vec{b} = b \cdot ( \text{BR}(\textcolor{red}{2},\textcolor{blue}{1})\hat{x} + \text{BR}(\textcolor{red}{2},\textcolor{blue}{2})\hat{y} + \text{BR}(\textcolor{red}{2},\textcolor{blue}{3})\hat{z} ) \\ \vec{c} = c \cdot ( \text{BR}(\textcolor{red}{3},\textcolor{blue}{1})\hat{x} + \text{BR}(\textcolor{red}{3},\textcolor{blue}{2})\hat{y} + \text{BR}(\textcolor{red}{3},\textcolor{blue}{3})\hat{z} ) \end{cases}$$

```
ftn58sparse.Ainfo
```

```
ans =
```

```
1x5 struct array with fields:
```

```
Atom  
Position  
Norb  
OrbitIndex  
Orbit  
OrbitID
```

```
struct2table(ftn58sparse.Ainfo)
```

```
ans =
```

```
5x6 table
```

fractional coordinates !  
(in basis of  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$ )

Atom	Position			Norb	OrbitIndex				Orbit				OrbitID			
'Bi'	0.399	0.399	0.399	4	1	2	3	4	' s px py pz'	1	2	3	4			
'Bi'	0.601	0.601	0.601	4	5	6	7	8	' s px py pz'	1	2	3	4			
'Se'	0	0	0	4	9	10	11	12	' s px py pz'	1	2	3	4			
'Se'	0.792	0.792	0.792	4	13	14	15	16	' s px py pz'	1	2	3	4			
'Se'	0.208	0.208	0.208	4	17	18	19	20	' s px py pz'	1	2	3	4			

ftn58sparse.Orbitps

OrbitIndex ans =	original OrbitIndex	Atom	Position			OrbitID
1.0000	1.0000	1.0000	0.3990	0.3990	0.3990	1.0000
2.0000	2.0000	1.0000	0.3990	0.3990	0.3990	2.0000
3.0000	3.0000	1.0000	0.3990	0.3990	0.3990	3.0000
4.0000	4.0000	1.0000	0.3990	0.3990	0.3990	4.0000
5.0000	5.0000	2.0000	0.6010	0.6010	0.6010	1.0000
6.0000	6.0000	2.0000	0.6010	0.6010	0.6010	2.0000
7.0000	7.0000	2.0000	0.6010	0.6010	0.6010	3.0000
8.0000	8.0000	2.0000	0.6010	0.6010	0.6010	4.0000
9.0000	9.0000	3.0000	0	0	0	1.0000
10.0000	10.0000	3.0000	0	0	0	2.0000
11.0000	11.0000	3.0000	0	0	0	3.0000
12.0000	12.0000	3.0000	0	0	0	4.0000
13.0000	13.0000	4.0000	0.7920	0.7920	0.7920	1.0000
14.0000	14.0000	4.0000	0.7920	0.7920	0.7920	2.0000
15.0000	15.0000	4.0000	0.7920	0.7920	0.7920	3.0000
16.0000	16.0000	4.0000	0.7920	0.7920	0.7920	4.0000
17.0000	17.0000	5.0000	0.2080	0.2080	0.2080	1.0000
18.0000	18.0000	5.0000	0.2080	0.2080	0.2080	2.0000
19.0000	19.0000	5.0000	0.2080	0.2080	0.2080	3.0000
20.0000	20.0000	5.0000	0.2080	0.2080	0.2080	4.0000
21.0000	1.0000	1.0000	0.3990	0.3990	0.3990	1.0000
22.0000	2.0000	1.0000	0.3990	0.3990	0.3990	2.0000