

```

scc.HubU=...           // U for each state, [state_label, U] or blank
[1,10;2,10;3,10;4,10;5,10;6,10;7,10;8,10;9,10;10,10]
scc.Charge=...         // charge of each state, 1x total state
[1,1,1,0,0,1,1,1,0,0,1,1,1,1,1,1]
scc.Mixing=[1]         // mixing parameter, 0~1
scc.Iteration=[30]     // maximal iterations, integer
scc.Converge=[10^-3]   // convergence criterion, real, at least < 0.1
scc.Mesh=[15,15,15]   // k-space mesh for Ef, (1x1,1x2,1x3), large for metal
scc.Temperature=[100]  // temperature for searching Ef, large for insulator
scc.Memory='max'       // 'normal', 'max', 'HDD' to store H_k

```

===== PiLib Variable =====

```

scc.E_Fermi, @full, the Fermi level
ORDER= 0, SIZE=[ 1, 1], TYPE=REAL

```

1

1.106961

===== PiLib Variable =====

```

scc.E_gap, @full, the band gap
ORDER= 0, SIZE=[ 1, 1], TYPE=REAL

```

1

4.677996

===== PiLib Variable =====

```

scc.DM_out, @t-sp, the output density matrix
ORDER= 1, SIZE=[ 17, 3], TYPE=SPARSE

```

1	2	3
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16	16	0.000000	0.000000
1	1	0.099891	0.000000
2	2	0.099868	0.000000
3	3	0.099865	0.000000
4	4	0.015352	0.000000
5	5	0.014631	0.000000
6	6	0.099891	0.000000
7	7	0.099868	0.000000
8	8	0.099865	0.000000
9	9	0.015352	0.000000
10	10	0.014631	0.000000
11	11	0.089999	0.000000
12	12	0.090280	0.000000
13	13	0.090114	0.000000
14	14	0.089999	0.000000
15	15	0.090280	0.000000
16	16	0.090114	0.000000

===== PiLib Variable =====

```

scc.U_mat, @t-sp, the Hubbard potential matrix
ORDER= 1, SIZE=[ 11, 3], TYPE=SPARSE

```

1	2	3
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