1 Introduction

ban is a task of application level. It can calculate band structure along a particular k-path. Because **ban** will output huge data. We will not attach all output in this file but just keep the output variable name. One may check any **ban** file in the examples for details.

2 Dictionary

2.1 Input

ban.Format This parameter tells PiLab how do you define the k-path. There are two options: 'coefficient' or 'coordinate'. Any k-point can be represented by $\mathbf{k} = c_1\mathbf{b}_1 + c_2\mathbf{b}_2 + c_3\mathbf{b}_3$. If 'coefficient', you input values in **ban.Path** will be interpreted as $[c_1, c_2, c_3]$. If 'coordinate', it will be interpreted as $[k_x, k_y, k_z]$. By default, this parameter is set 'coefficient'.

ban.Path This parameter defines the k-path. The k-path is defined by connecting many k-points. So just input all the k-points you want to go through, PiLab will automatically generate k-mesh along these path.

ban.Div This parameter defines how many k-points between two input k-points.

ban.DivType This parameter tells PiLab how to divide each k-path. 'unit' or 'all'. If 'unit', it divide each unit length in k-space into ban.Div k-points. If 'all', it divide a whole k-path, e.g $[0, 0, 0]$ to $[1, 1, 1]$ into ban.Div k-points. Note that, the length of k-space are defined by the reciprocal lattice times lattice constant. Therefore all axis ranges from 0 to 2π. So the are independent of lattice constant.

ban.Draw This parameter tells PiLab whether you want to draw band structures. 'on' or 'off'. Default value is 'on'.

ban.Shift This parameter tells PiLab whether you want to shift Fermi level to zero in the band structure plot. Note that, this is just a shift in the plot. The original data will not be changed.

2.2 Output

ban.k_path_div This variable tells how many k-points are generated in each k-path.

ban.k_point This variable lists all k-points. Each row vector contains 4 elements [label, k_x, k_y, k_z]. The first just shows it is the n-th k-point.

ban.k_band This variable shows the band energies. Each column vector is the band energies of a particular k-point. For example, if there are 100 k-point in total and each k-point has 10 energy levels. Then it would be a 10x100 matrix. The n-th column is the band energies of the n-th k-point shown in ban.k_point.

ban.k_vec(:,:,n) This is the eigenvector matrix of the n-th k-point. Also, if there are 10 bands at each k-point, it would be a 10x10 matrix.

```
ban.Format=['coefficient']        // 'coefficient' or 'coordinate'
ban.Path=...                      // points to defined your paths, nx3/nx2,nx1
[0,0,0;1/2,1/2,1/2;1/2,0,0;0,1/2,0;0,0,1/2;0,0,0]
ban.Div=[40]                      // k points of each path
ban.DivType='unit'                // how to divide k_path, 'unit' or 'all'
ban.Draw=['on']                   // whether draw band structure, 'on' or 'off'
ban.Shift=['on']                  // whether shift Ef to 0 in band plot, 'on' or 'off

============== PiLib Variable ==============
ban.k_path_div, @full, number of division of each path
ORDER=    0, SIZE=[    5,    1], TYPE=INTEGER

============== PiLib Variable ==============
ban.k_point, @full, [label,kx,ky,kz]
ORDER=    2, SIZE=[  200,    4], TYPE=REAL


============== PiLib Variable ==============
ban.k_band, @full, [En(k1),En(k2)...]
ORDER=    0, SIZE=[   16,  200], TYPE=REAL


============== PiLib Variable ==============
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Figure 1: page 1 of NiO_ban.plb