
pyramids Documentation

Release

Author

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pyramids package

Subpackages

pyramids.io package

Submodules

pyramids.io.fdf module

Created on Fri July 22 18:16:20 2016 The collection of the useful methods used in the TDAP results analysis

```
class pyramids.io.fdf.tdapOptions (inputFile='input.fdf')
    Bases: object
        getFloat (label, default)
        getFloatWithUnit (label, default)
        getInteger (label, default)
        getLogical (label, default)
        getString (label, default)
        output ()
        readFdf (inputFile='input.fdf')
```

pyramids.io.output module

Created on Wed Jul 27 00:10:57 2016

@author: clian

```
pyramids.io.output.writeSiesta (filename, atoms)
```

pyramids.io.result module

Created on Mon Jul 25 20:28:55 2016 The collection of the useful methods used in the TDAP results analysis

```
pyramids.io.result.getBands (bandType='e')
    return the bands read from systemLabel.bands as the dimension numKpoint x numBand x numSpin returns: X,
    Ek, xticks, xticklabels
```

```
pyramids.io.result.getBerry (step='')  
    return the Eigenvalues read from systemLabel.EIG  
pyramids.io.result.getDOS (filename='siesta.dos')  
    return the dos read from filename as the dimension numEnergyPoint returns: energy, up, down, total  
pyramids.io.result.getDipole()  
pyramids.io.result.getEField()  
pyramids.io.result.getEIGSteps()  
pyramids.io.result.getEigAndPar (timeSteps=None, forceReread=False)  
    return the Times, Eigvalues and Partitions at selected timeSteps write two files EIG and PAR  
pyramids.io.result.getEnergyTemperaturePressure()  
    return the Temperature, KS Energy and Total Energy as the dimension of Nstep read from systemLabel.MDE  
    returns the Temperature, KS Energy, Total Energy, Volume, Pressure  
pyramids.io.result.getExcitedElectrons (selectK=None)  
pyramids.io.result.getFermiEnergy()  
    return the Fermi Energy read from systemLabel.EIG if failed, return 0 rather than raise an exception  
pyramids.io.result.getHomo()  
    return the index of the highest occupied molecular orbital (HOMO)  
pyramids.io.result.getTrajectory()  
pyramids.io.result.loadSaved (filename)  
pyramids.io.result.readEigFile (filename='')  
    return the Eigenvalues read from systemLabel.EIG
```

Module contents

pyramids.plot package

Submodules

pyramids.plot.PlotUtility module

pyramids.plot.setting module

Created on Fri Jan 22 18:16:20 2016 The collection of the useful methods used in the TDAP results analysis

```
pyramids.plot.setting.getColors (colorList, cmap='jet')  
pyramids.plot.setting.getPropertyFromPosition (index=None, xlabel='', ylabel='',  
                                                title='', xticks=None, yticks=None, xtick-  
                                                labels=None, yticklabels=None, xlim-  
                                                its=None, ylimits=None, hline=None,  
                                                vline=None)  
    a utility function to set the property of the figure axe  
pyramids.plot.setting.setProperty (ax, **kargs)  
    a utility function to set the property of the figure axe
```


Module contents

pyramids.process package

Submodules

pyramids.process.struct module

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