NAME

>Psi4Util

SYNOPSIS

>import Psi4Util

DESCRIPTION

>Psi4Util module provides the following functions:

>CalculateSinglePointEnergy, GetAtomPositions, InitializePsi4, JoinMethodNameAndBasisSet, ListPsi4RunParamaters, PerformGeometryOptimization, ProcessPsi4ConstrainTorsionsParameters, ProcessPsi4CubeFilesParameters, ProcessPsi4DDXSolvationParameters, ProcessPsi4OptionsParameters, ProcessPsi4RunParameters, RemoveScratchFiles, RetrieveIsocontourRangeFromCubeFile, RetrieveMinAndMaxValueFromCubeFile, SetupPsi4DDXSolvationOptions, UpdatePsi4OptionsParameters, UpdatePsi4OutputFileUsingPID, UpdatePsi4RunParameters

FUNCTIONS

>CalculateSinglePointEnergy

>>CalculateSinglePointEnergy(psi4, Molecule, Method, BasisSet, ReturnWaveFunction = False, Quiet = False)

>Calculate single point electronic energy in Hartrees using a specified method and basis set.

>*Arguments:*

```
psi4 (Object): Psi4 module reference.
Molecule (Object): Psi4 molecule object.
Method (str): A valid method name.
BasisSet (str): A valid basis set.
ReturnWaveFunction (bool): Return wave function.
Quiet (bool): Flag to print error message.
```

>*Returns:*

```
float: Total electronic energy in Hartrees.
(float, psi4 object): Energy and wavefuction.
```

>GetAtomPositions

>>GetAtomPositions(psi4, WaveFunction, InAngstroms = True)

>Retrieve a list of lists containing coordinates of all atoms in the molecule available in Psi4 wave function. By default, the atom positions are returned in Angstroms. The Psi4 default is Bohr.

>*Arguments:*

```
psi4 (Object): Psi4 module reference.
WaveFunction (Object): Psi4 wave function reference.
InAngstroms (bool): True - Positions in Angstroms; Otherwise, in Bohr.
```

>*Returns:*

```
None or list : List of lists containing atom positions.
```

>*Example(s):*

```
for AtomPosition in Psi4Util.GetAtomPositions(Psi4Handle, WaveFunction):
    print("X: %s; Y: %s; Z: %s" % (AtomPosition[0], AtomPosition[1],
        AtomPosition[2]))
```

>InitializePsi4

>>InitializePsi4(Psi4RunParams = None, Psi4OptionsParams = None, PrintVersion = False, PrintHeader = False)

>Import Psi4 module and configure it for running Psi4 jobs.

Arguments:

```
Psi4RunParams (dict): Runtime parameter name and value pairs.
Psi4OptionsParams (dict): Option name and value pairs. This is simply
    passed to ps4.set_options().
PrintVersion (bool): Print version number.
PrintHeader (bool): Print header information.
```

Returns:

```
Object: Psi4 module reference.
```

JoinMethodNameAndBasisSet

```
JoinMethodNameAndBasisSet(MethodName, BasisSet)
```

Join method name and basis set using a backslash delimiter. An empty basis set specification is ignored.

Arguments:

```
MethodName (str): A valid method name.
BasisSet (str): A valid basis set or an empty string.
```

Returns:

```
str: MethodName/BasisSet or MethodName
```

ListPsi4RunParamaters

```
ListPsi4RunParamaters(psi4)
```

List values for a key set of the following Psi4 runtime parameters: Memory, NumThreads, OutputFile, ScratchDir, DataDir.

Arguments:

```
psi4 (object): Psi4 module reference.
```

Returns:

```
None
```

PerformGeometryOptimization

```
PerformGeometryOptimization(psi4, Molecule, Method, BasisSet, ReturnWaveFunction =
True, Quiet = False)
```

Perform geometry optimization using a specified method and basis set.

Arguments:

```
psi4 (Object): Psi4 module reference.
Molecule (Object): Psi4 molecule object.
Method (str): A valid method name.
BasisSet (str): A valid basis set.
ReturnWaveFunction (bool): Return wave function.
Quiet (bool): Flag to print error message.
```

Returns:

```
float: Total electronic energy in Hartrees.
(float, psi4 object): Energy and wavefuction.
```

ProcessPsi4ConstrainTorsionsParameters

```
ProcessPsi4ConstrainTorsionsParameters(ParamsOptionName, ParamsOptionValue,
ParamsDefaultInfo = None)
```

Process parameters for Psi4 constrain torsions around rotatable bonds and return a map containing processed parameter names and values.

ParamsOptionValue is a comma delimited list of parameter name and value pairs for generating cube files.

The supported parameter names along with their default and possible values are shown below:

ignoreHydrogens, yes, rotBondsSMARTSMode, NonStrict, rotBondsSMARTSPattern, Auto

Arguments:

```
ParamsOptionName (str): Command line Psi4 constrain torsions option name.
ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.
ParamsDefaultInfo (dict): Default values to override for selected parameters.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

ProcessPsi4CubeFilesParameters

```
ProcessPsi4CubeFilesParameters(ParamsOptionName, ParamsOptionValue, ParamsDefaultInfo =
None)
```

Process parameters for Psi4 runs and return a map containing processed parameter names and values.

ParamsOptionValue is a comma delimited list of parameter name and value pairs for generating cube files.

The supported parameter names along with their default and possible values are shown below:

GridSpacing, 0.2, GridOverage, 4.0, IsoContourThreshold, 0.85

GridSpacing: Units: Bohr. A higher value reduces the size of the cube files on the disk. This option corresponds to Psi4 option CUBIC_GRID_SPACING.

GridOverage: Units: Bohr.This option corresponds to Psi4 option CUBIC_GRID_OVERAGE.

IsoContourThreshold captures specified percent of the probability density using the least amount of grid points. This option corresponds to Psi4 option CUBEPROP_ISOCONTOUR_THRESHOLD.

Arguments:

```
ParamsOptionName (str): Command line Psi4 cube files option name.
ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.
ParamsDefaultInfo (dict): Default values to override for selected parameters.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

ProcessPsi4DDXSolvationParameters

```
ProcessPsi4DDXSolvationParameters(ParamsOptionName, ParamsOptionValue,
ParamsDefaultInfo = None)
```

Process parameters for Psi4 DDX solvation and return a map containing processed parameter names and values.

ParamsOptionValue is a space delimited list of parameter name and value pairs for solvation energy calculations.

The supported parameter names along with their default and possible values are shown below:

SolvationModel PCM Solvent water solventEpsilon None radiiSet UFF

solvationModel: Solvation model for calculating solvation energy. The corresponding Psi4 option is DDX_MODEL.

solvent: Solvent to use. The corresponding Ps4 option is DDX_SOLVENT.

solventEpsilon: Dielectric constant of the solvent. The corresponding Psi4 option is DDX_SOLVENT_EPSILON.

radiiSet: Radius set for cavity spheres. The corresponding Psi option is DDX_RADII_SET.

Arguments:

```
ParamsOptionName (str): Command line Psi4 DDX solvation option name.
ParamsOptionValues (str): Space delimited list of parameter name and value pairs.
ParamsDefaultInfo (dict): Default values to override for selected parameters.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

ProcessPsi4OptionsParameters

```
ProcessPsi4OptionsParameters(ParamsOptionName, ParamsOptionValue)
```

Process parameters for setting up Psi4 options and return a map containing processed parameter names and values.

ParamsOptionValue is a comma delimited list of Psi4 option name and value pairs for setting global and module options. The names are 'option_name' for global options and 'module_name__option_name' for options local to a module. The specified option names must be valid Psi4 names. No validation is performed.

The specified option name and value pairs are processed and passed to psi4.set_options() as a dictionary. The supported value types are float, integer, boolean, or string. The float value string is converted into a float. The valid values for a boolean string are yes, no, true, false, on, or off.

Arguments:

```
ParamsOptionName (str): Command line input parameters option name.
ParamsOptionValue (str): Comma delimited list of parameter name and value pairs.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

ProcessPsi4RunParameters

```
ProcessPsi4RunParameters(ParamsOptionName, ParamsOptionValue, InfileName = None,
ParamsDefaultInfo = None)
```

Process parameters for Psi4 runs and return a map containing processed parameter names and values.

ParamsOptionValue a comma delimited list of parameter name and value pairs for configuring Psi4 jobs.

The supported parameter names along with their default and possible values are shown below:

MemoryInGB,1,NumThreads,1,OutputFile,auto,ScratchDir,auto, RemoveOutputFile,yes

Possible values: OutputFile - stdout, quiet, or FileName; ScratchDir - DirName; RemoveOutputFile - yes, no, true, or false

These parameters control the runtime behavior of Psi4.

The default for 'OutputFile' is a file name <InFileRoot>_Psi4.out. The PID is appened the output file name during multiprocessing. The 'stdout' value for 'OutputType' sends Psi4 output to stdout. The 'quiet' or 'devnull' value suppresses all Psi4 output.

The default 'Yes' value of 'RemoveOutputFile' option forces the removal of any existing Psi4 before creating new files to append output from multiple Psi4 runs.

The option 'ScratchDir' is a directory path to the location of scratch files. The default value corresponds to Psi4 default. It may be used to override the deafult path.

Arguments:

```
ParamsOptionName (str): Command line Psi4 run parameters option name.
ParamsOptionValues (str): Comma delimited list of parameter name and value pairs.
InfileName (str): Name of input file.
ParamsDefaultInfo (dict): Default values to override for selected parameters.
```

Returns:

```
dictionary: Processed parameter name and value pairs.
```

The parameter name and values specified in ParamsOptionValues are validated before returning them in a dictionary.

RemoveScratchFiles

```
RemoveScratchFiles(psi4, OutputFile, PID = None)
```

Remove any leftover scratch files associated with the specified output file. The file specification,

<OutfileRoot>.*<PID>.* is used to collect and remove files from the scratch directory. In addition, the file psi.<PID>.clean, in current directory is removed.

Arguments:

```
psi4 (object): psi4 module reference.
OutputFile (str): Output file name.
PID (int): Process ID or None.
```

Returns:

```
None
```

RetrieveIsocontourRangeFromCubeFile

```
RetrieveIsocontourRangeFromCubeFile(CubeFileName)
```

Retrieve isocontour range values from the cube file. The range values are retrieved from the second line in the cube file after the string 'Isocontour range'.

Arguments:

```
CubeFileName (str): Cube file name.
```

Returns:

```
float: Minimum range value.
float: Maximum range value.
```

RetrieveMinAndMaxValueFromCubeFile

```
RetrieveMinAndMaxValueFromCubeFile(CubeFileName)
```

Retrieve minimum and maxmimum grid values from the cube file.

Arguments:

```
CubeFileName (str): Cube file name.
```

Returns:

```
float: Minimum value.
float: Maximum value.
```

SetupPsi4DDXSolvationOptions

```
SetupPsi4DDXSolvationOptions(SolvationMode, ParamsInfo)
```

Setup Psi4 options for calculating solvation energy using DDX module.

Arguments:

```
SolvationMode (bool): Set DDX option for solvation calculation.
ParamsInfo (dict): Psi4 DDX parameter name and value pairs.
```

Returns:

```
dictionary: Psi4 Option name and value pairs.
```

UpdatePsi4OptionsParameters

```
UpdatePsi4OptionsParameters(psi4, OptionsInfo)
```

Update Psi4 options using psi4.set_options().

Arguments:

```
psi4 (object): Psi4 module reference.
OptionsInfo (dictionary) : Option name and value pairs for setting
    global and module options.
```

Returns:

```
None
```

UpdatePsi4OutputFileUsingPID

```
UpdatePsi4OutputFileUsingPID(OutputFile, PID = None)
```

Append PID to output file name. The PID is automatically retrieved during None value of PID.

Arguments:

```
OutputFile (str): Output file name.
PID (int): Process ID or None.
```

Returns:

```
str: Update output file name. Format: <OutFieRoot>_<PID>.<OutFileExt>
```

UpdatePsi4RunParameters

```
UpdatePsi4RunParameters(psi4, RunParamsInfo)
```

Update Psi4 runtime parameters. The supported parameter names along with their default values are as follows: MemoryInGB: 1; NumThreads: 1, OutputFile: stdout; ScratchDir: auto; RemoveOutputFile: True.

Arguments:

```
psi4 (object): Psi4 module reference.
RunParamsInfo (dictionary) : Parameter name and value pairs for
    configuring Psi4 jobs.
```

Returns:

```
None
```

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