ecx

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NAME

ecx - library for electrochemistry

SYNOPSIS

use *ecx*

DESCRIPTION

ecx a Fortran library for providing a collection of routines for electrochemistry. A C API allows usage from C, or can be used as a basis for other wrappers. A Python wrapper allows easy usage from Python.

It covers:

> **o kinetics**
> > Nernst, Butler-Volmer
>
> **o electrochemical**
> > Impedance, Admittance, Circuit Elements, Equivalent Circuits
>
> **o photoelectrochemistry**
> > Photocurrent, Band-gap, space charge.

The C API is defined by adding a prefix to the functions from the Fortran API due to the lack of module/namespace feature in the C language. The functions are therefore following this template: (c_prefix)fortran_func.

- (ecx_)get_version
- (ecx_core_)kTe
- (ecx_eis_)z
- mm
- (ecx_kinetics_)nernst
- (ecx_kinetics_)sbv
- (ecx_kinetics_)bv
- (ecx_eis_)z

EXAMPLE

Minimal example in Fortran:

```
use ecx
```

Minimal example in C:

```
include "ecx.h"
```

Minimal example in Python:

```
import pyecx
```

SEE ALSO

complex(7), **gsl**(3), **catanh**(3), **gnuplot**(1)

[0%]   ecx_api.f90

[11%] ecx_api.f90 done.

[11%] ecx_capi.f90

[22%] ecx_capi.f90 done.

[22%] ecx.f90

[33%] ecx.f90 done.

[33%] libecx.a

[44%] libecx.a done.

[44%] main.f90

[55%] main.f90 done.

[55%] example.f90

[66%] example.f90 done.

[66%] ecxcli

[77%] ecxcli done.

[77%] example_in_c

[88%] example_in_c done.

[88%] example_in_f

[100%]

example_in_f done. [100%] Project compiled successfully.

NAME

ecxcli(1) - Command line for ecx

SYNOPSIS

ecxcli *SUBCOMMAND* [*OPTIONS ...*] *ARGS ...*

DESCRIPTION

ecxcli is command line interface for computing electro- chemical properties:

     o EIS   Electrochemical Impedance **Z=f**(w)

     o Kinetics

         j=f(U)

     o PEC   **Iph=f**(hv, U)

It can also provide the molar masses, isotope compositions and nuclide compositions.

SUBCOMMANDS

     o all   Get the whole periodic table.

     o saw   Get the standard atomic weight.

Enter **ecxcli** *SUBCOMMAND* **--help** for detailed descriptions.

OPTIONS

     o --abridged, -a

         Use the abridged value.

     o --uncertainty, -u

         Use the uncertainty.

      o --pprint
           Nice formatting.

      o --mass, -z
           Get the mass number.

VALID FOR ALL SUBCOMMANDS

      o --help
           Show help text and exit

      o --verbose
           Display additional information when available.

      o --version
           Show version information and exit.

NAME

　　　　get_version - version getter for the library

LIBRARY

　　　　Electrochemistry library - (**-libecx**, **-lecx**)

SYNOPSIS

　　　　get_version()

DESCRIPTION

　　　　This function returns the version of the ecx library.

RETURN VALUE

　　　　character(len=:), pointer :: fptr

NAME
 kTe - thermal voltage

SYNOPSIS
 kTe(*T*)

DESCRIPTION
 Compute the thermal voltage.

 Parameters:

 o *T*   Temperature in Â°C

RETURN VALUE
 real(dp) :: r
 Thermal voltage in Volts.