**Opium - pseudopotential generation project**

* From the Computing[MTU] Showcase Workshop: [**Examining the Aufbau Principle through Computational Chemistry**](https://www.mtu.edu/icc/events/computing-showcase/showcase-workshops/#metz) with Dr. Irene Metz: April 5, 1:45-3 p.m. and April 6, 9-11 a.m.

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| **Disclaimer**: Opium is distributed under the [GNU General Public Licence](http://www.gnu.org/copyleft/gpl.txt). Like most open source software, it is not guaranteed to be bug free. Use at your own risk and please report any bugs to the Opium [mailing list](http://sourceforge.net/mailarchive/forum.php?forum_id=10457).**Latest release**[Version 4.1](http://sourceforge.net/projects/opium/files/opium/opium-v4.1)- April 10, 2018View the [4.0 -> 4.1 Changelog](http://opium.sourceforge.net/changelog4.1.txt)View the [FULL Changelog](http://opium.sourceforge.net/changelog.txt)Get the *Emacs highlighting mode* [here](http://opium.sourceforge.net/_emacs_mode)**Scientific background / Features**The ab initio pseudopotential method is now a well established tool in condensed matter physics, computational chemistry and material science. At the present time there are a good number of codes available, both commercial and in the public domain, that perform electronic structure calculations of molecules and solids based on the pseudopotential scheme. The most important input information that these programs require are the pseudopotentials used in the calculation.Features included in the current release of Opium:* Scalar-relativistic [[1](http://opium.sourceforge.net/sci.html#bib:igrel)] and non-relativistic pseudopotential generation
* Ability to construct Optimized (RRKJ) [[2](http://opium.sourceforge.net/sci.html#bib:rrkj)] or Kerker [[3](http://opium.sourceforge.net/sci.html#bib:kerker)] pseudopotentials
* Partial core correction of Louie, Froyen and Cohen [[4](http://opium.sourceforge.net/sci.html#bib:lfc)]
* Can test and generate and test pseudopotentials that support semicore states
* Ghost state checking following the method suggested by Gonze, Stumpf, and Scheffler [[5](http://opium.sourceforge.net/sci.html#bib:ghosts)]
* Automatic plotting of wavefunctions, potentials, and density using [xmgrace](http://plasma-gate.weizmann.ac.il/Grace/)
* Implementation of the designed non-local potential approach of Ramer and Rappe [[6](http://opium.sourceforge.net/sci.html#bib:dnl)].

**Computational packages that are currently supported by Opium output formats**

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| **Format** | **Package** |
| \*.upf | [Quantum ESPRESSO](http://www.quantum-espresso.org/) |
| \*.recpot | [CASTEP](http://www.cse.clrc.ac.uk/cmg/NETWORKS/UKCP/) |
| \*.fhi | [ABINIT](http://www.abinit.org/) | [JDFTx](http://jdftx.sourceforge.net/) |
| \*.ncpp | [PWSCF](http://www.pwscf.org/) |  |
| \*.pwf | Bh |  |
| \*.cpi | [FHI98md](http://www.fhi-berlin.mpg.de/th/fhi98md/index.html) |  |

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| **Last updated: Apr 10, 2018** |

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