SIESTA

Acknowledging

The Licensee is also requested to cite the following papers in any document issued by the Centre that refers to the SIESTA package:

1. “Self-consistent order-N density-functional calculations for very large systems”, P. Ordejón, E. Artacho and J. M. Soler, Phys. Rev. B (Rapid Comm.) 53, R10441-10443 (1996).
2. “The SIESTA method for ab initio order-N materials simulation” J. M. Soler, E. Artacho,J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matt. 14, 2745-2779 (2002).

Other papers relevant to the SIESTA package and method can also be cited as best scientific practice dictates. Licensees are recommended to send reference to the Developers of any publication containing results wholly or partially derived from the results of use of the SIESTA package.

User validation for Computer Centres

If you want to use SIESTA for commercial work please ask us.

We have simplified the procedure for access to the Siesta code for academic users: they can now proceed directly to the download area by explicitly accepting the licensing conditions, without a formal registration.

Computer centres with an installed Siesta executable were formerly required to check whether a person was a registered Siesta user before granting access to the executable. We suggest that a simpler test for academic affiliation is used instead (for example, a web interface in which the prospective user can click a box declaring academic affiliation). In case of doubt, please email to siesta at uam.es, with the subject "Computer center check".

Using SIESTA on Blue Wonder

Here is a very simple job submission script for the H2O example on the iDataPlex. This assumes you have already generated the H and O pseudo-potentials. See the user manual in /gpfs/packages/intel/siesta/3.1/Docs .

```
#BSUB -J SIESTA
#BSUB -o stdout.%J.txt
#BSUB -e stderr.%J.txt
#BSUB -R "span[ptile=16]"
#BSUB -n 32
```

```
#BSUB -W 0:20

cd $LS_SUBCWD

#Load modules
source /etc/profile.d/modules.sh
module load siesta/3.1

export myexe="siesta"

#execute SIESTA
mpiexec.hydra -np 32 $myexe < h2o.fdf
```

Further Information

See http://icmab.cat/leem/siesta/ . User documentation and tutorials are here: http://departments.icmab.es/leem/siesta/Documentation/index.html .