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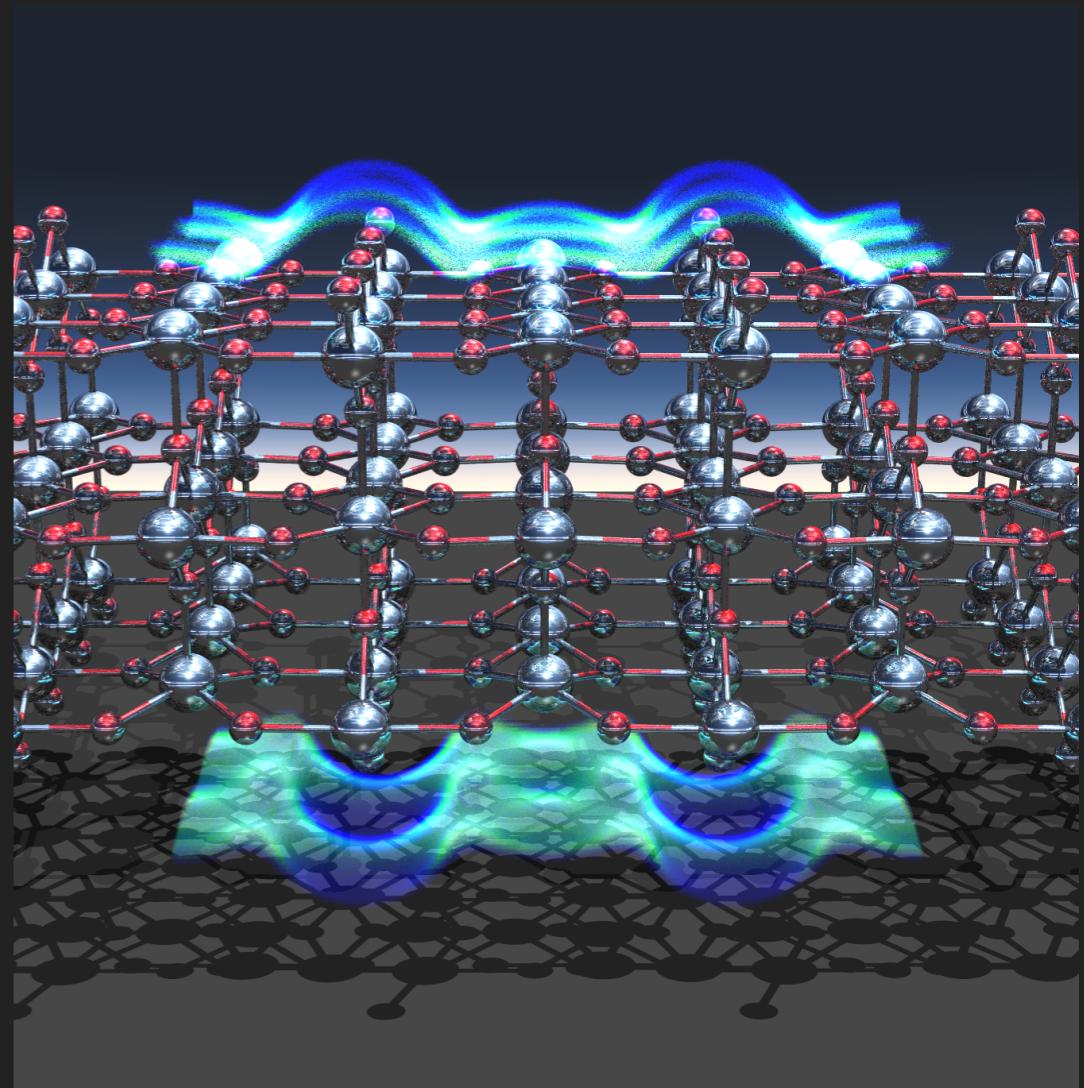
[www.materialab.org](http://www.materialab.org)

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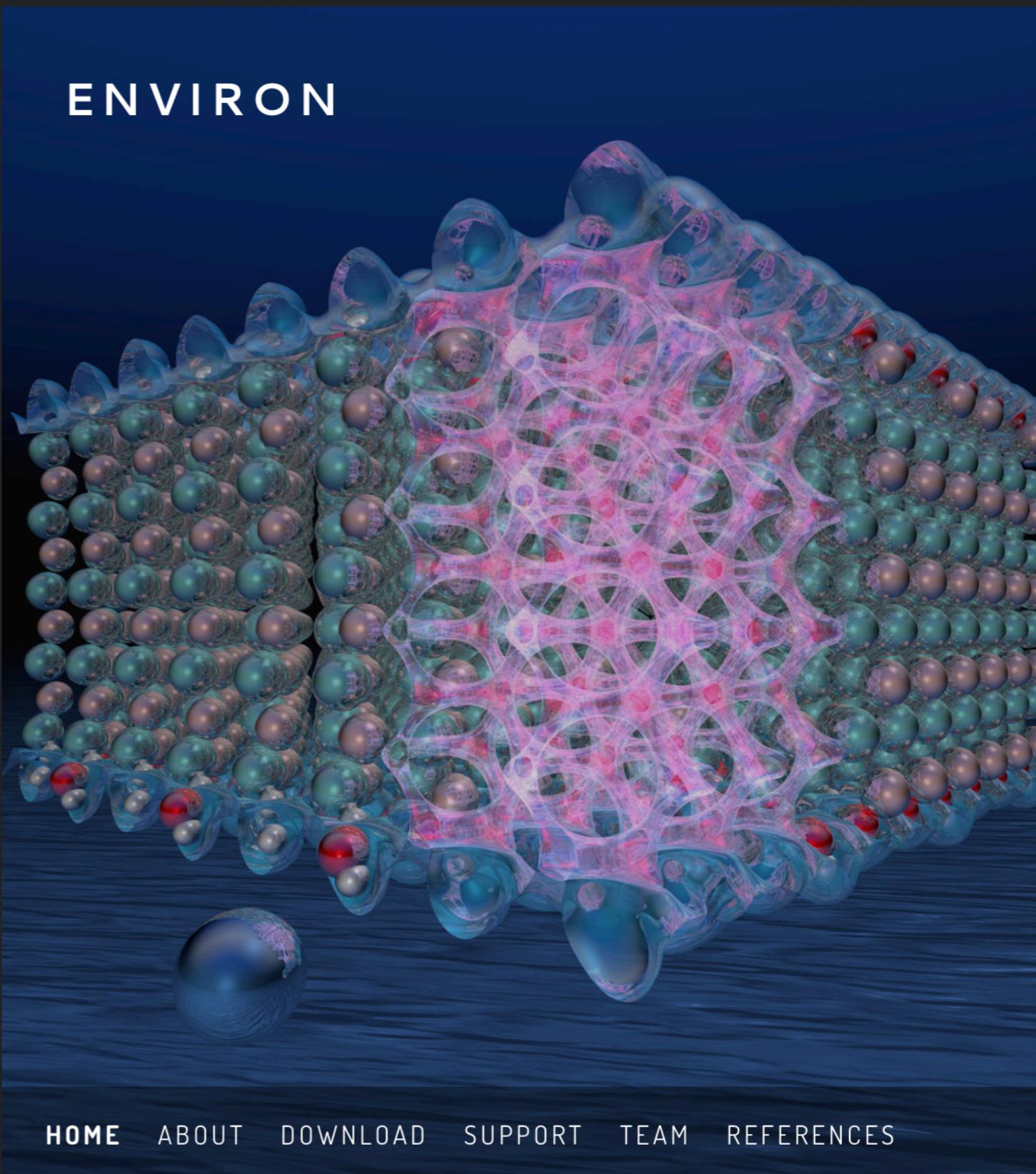
# **ENVIRON: CONTINUUM EMBEDDINGS IN QUANTUM-ESPRESSO**

**I-COMSE SUMMER SCHOOL 06/04/23-06/08/23**



## THE CODE

- Basic information
- Download and installation
- Input and Output
- Testing and examples



## AN OPEN SOURCE PROJECT

- ▶ Website: [www.quantum-environ.org](http://www.quantum-environ.org)
- ▶ Documentation: <https://environ.readthedocs.io>
- ▶ Public Q&A group: [quantum-environ-users@googlegroups.com](mailto:quantum-environ-users@googlegroups.com)
- ▶ Public GitHub mirror: <https://github.com/environ-developers/Environ>
  
- ▶ Six main releases:
  - ▶ Environ 0.1 in February 2015
  - ▶ Environ 0.2 in February 2016
  - ▶ Environ 1.0 in February 2018
  - ▶ Environ 1.1 in April 2019
  - ▶ Environ 2.0 in October 2021
  - ▶ Environ 3.0 in July 2022

## ENVIRON 3.0

- ▶ A modular library written in Fortran 90/95/2003
- ▶ It exploits reciprocal-space operations (FFTs) for numerical intense tasks (gradients, Poisson potential, and related stuff)
- ▶ Compiled as a stand-alone library
  - ▶ Can be used as a post-processing tool on cubefiles
  - ▶ Clean API to interface it with other codes
  - ▶ Currently coupled with QE (working on FHI-aims and Dlpoly)
- ▶ Extended use of object-oriented principles

## DOWNLOAD AND INSTALLATION

- ▶ For news and releases, check out
  - ▶ [www.quantum-environ.org](http://www.quantum-environ.org)
- ▶ For installation instructions, theoretical overview, and more, check out
  - ▶ <https://environ.readthedocs.io/en/latest/>
- ▶ Instructions are also available in the README file
- ▶ Once installed:
  1. Run the test-suite to check for consistency
  2. Run the examples to get familiarized with the tools
  3. Input keywords are also in Doc/INPUT\_Environ.html

### INPUT FILE

- ▶ Environ requires one additional input file
- ▶ It must be named **environ.in** and located in the directory where pw.x is running
- ▶ **environ.in** is composed of three namelists (two optional) and two optional cards

# ENVIRON NAMELISTS

## &ENVIRON (REQUIRED)

The global properties of the calculation

- ▶ The strength of the different environment effects
- ▶ Basic control keywords (verbosity)

## &BOUNDARY (OPTIONAL)

The definition of the continuum boundaries

## &ELECTROSTATIC (OPTIONAL)

The parameters for the electrostatic solvers

# ENVIRON CARDS

## **EXTERNAL\_CHARGES** (OPTIONAL)

- ▶ Defines additional charge densities included in the electronic structure calculation (must be activated by env\_external\_charges = N>0)

## **DIELECTRIC\_REGIONS** (OPTIONAL)

- ▶ Defines non-homogenous dielectric regions inside the simulation cell
- ▶ (must be activated by env\_dielectric\_regions = N>0)

# MULTIPLE LEVELS OF OUTPUT

### 1. verbose=0 (default)

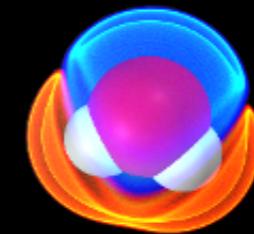
- ▶ only print minimal information to standard output (inside the QE output file)

### 2. verbose>0

- ▶ generate an additional readable text file named `environ.debug`
- ▶ contains information of the Environ calculations

### 3. verbose>1

- ▶ generate additional cube files
- ▶ contains values of specific physical quantities on the simulation grid



Cube files may be useful for debugging or rendering purposes; they can be viewed with molecular visualization software, such as VMD

# RUNNING TESTS

- ▶ Environ comes with a test-suite to allow for consistency checks
- ▶ To run the tests in serial, switch over to Environ/tests and run
  - ▶ make run-tests
- ...or in parallel
  - ▶ make run-tests-parallel

NOTE: a few tests may give some small errors and reported as failed

# RUNNING EXAMPLES

- ▶ Summarized in Environ/examples/README
  - ▶ To run, switch over to Environ/examples
1. Change directory into one of the examples
    - ▶ `cd example01/`
  2. Run the script
    - ▶ `./run_example.sh`
  3. Make sure the script to run the example is executable. If not, run
    - ▶ `chmod a+x run_example.sh`
  4. Compare results against the available references

# COUPLING WITH QE

- ▶ Environ is coupled with the following QE sub-packages:
  - ▶ PW & NEB
  - ▶ CP
  - ▶ TDDFPT
  - ▶ XSPECTRA
- ▶ To run environ with these codes, run (e.g. PW)
  - ▶ `$QEPATH/bin/pw.x -environ <filename.in > filename.out`

# STAND-ALONE DRIVER

- ▶ New Environ/programs folder
- ▶ ‘make’ will generate a driver executable
- ▶ ‘make usage name=from\_cube’ for instructions on how to run Environ as a post-processing tool on cubefiles.

# USERS & ENVIRON

- ▶ If you use the code and it works...
  - ▶ please cite the main references
  - ▶ full list available online and in the calculation output
- ▶ If you use the code and it doesn't work...
  - ▶ Bug - NO WORRIES!... we'll fix it
  - ▶ Numerical problems - GREAT!... Try tweaking the parameters
  - ▶ Physical problem - NOT SO GREAT! May require development of new features
- ▶ In any case, please:
  - ▶ Check out the FAQ online or the Q&A group
  - ▶ Contact us ([oliviero.andreussi@unt.edu](mailto:oliviero.andreussi@unt.edu))