

## CUBES: a library and a program suite for manipulating orbitals and densities

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### Abstract

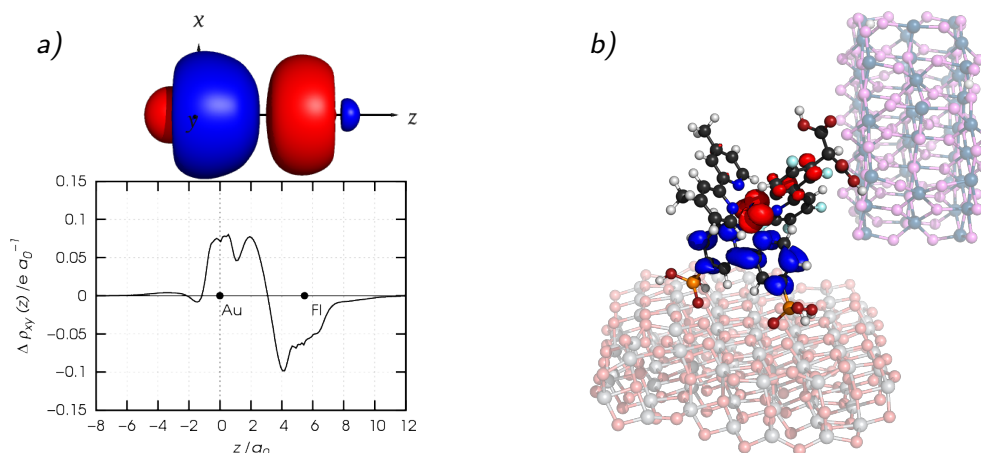
CUBES is a toolkit for manipulating 'cube' files storing quantum-chemical volumetric data such as molecular orbitals or electron densities. Written in modern Fortran, CUBES is both a library and a program suite providing a 'cube' data type, procedures for operating on it and ready-to-use commands for basic operations including read/write, add/subtract, multiply and integrate.

Chemical processes such as bond formation or electron excitation are often interpreted in terms of the changes that the total electron density undergoes in going from a reference (unbound or ground) state to the final (bound or excited) one. Pioneering in this respect have been Bader's late-Sixties studies on bonding in diatoms [1]. Electron densities and molecular orbitals, out of which the formers are built, are both the outcome of molecular electronic-structure calculations performed with several commercial and non-commercial packages such as Gaussian, Dalton, ADF and Molpro. On the computer side, these quantities are either represented as vectors or matrices reflecting their expansion in a basis set of known functions or discretised onto a finite-volume regular grid in physical space and saved into so-called 'cube' files (.cub or .cube extensions) interfaced with most visualization programs including Molden, Chimera and PyMOL.

Both a library and a program suite, CUBES (<http://www.srampino.com/code.html>) is a toolkit for manipulating cube files. The library provides a 'cube' data type and procedures for operating on it (such as read, write, access data, add, integrate and many others). The program suite is built on top of the library and provides ready-to-use commands for a manifold of basic operations such as add, subtract, multiply and integrate.

The ready-to-use commands are meant to be executed from command line and take as arguments directly the cube files. Eg, given two cube files `rho_xs.cube` and `rho_gs.cube` storing the electron densities of an excited and a ground state, respectively, a command as simple as

```
$ cubesub rho_xs.cube rho_gs.cube drho.cube
```



Two examples of density-difference analysis carried out with CUBES: a) charge rearrangement (red lobe: depletion, blue lobe: accumulation) and its profile along the interaction axis  $z$  (integrating over the normal  $xy$  planes) upon bond formation between superheavy element FI ( $Z = 114$ ) and Au [2] computed by four-component relativistic DFT [3] b) HOMO-LUMO density difference for a Ru(II) dye sensitizing a  $\text{TiO}_2$ -based solar cell (Dr Mariachiara Pastore and Dr Filippo De Angelis are gratefully acknowledged for providing the figure in this panel) [4].

will output a `drho.cube` file storing the density difference between the two states. The same command has been used to generate the cube files plotted in the figure as isodensity surfaces.

CUBES is written in modern Fortran (F standard: [http://www.fortran.com/F/F\\_bnf.html](http://www.fortran.com/F/F_bnf.html)) and features a minimal set of requirements: a Fortran 90/95 compiler and a Unix-like shell terminal.

## References

- [1] R F W Bader, W H Henneker, and Paul E Cade. [Molecular Charge Distributions and Chemical Binding](#). *The Journal of Chemical Physics*, 46:3341–3363, 1967.
- [2] S Rampino, L Storchi, and L Belpassi. [Gold–superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study](#). *The Journal of Chemical Physics*, 143:024307 (8 pp.), 2015.
- [3] S Rampino, L Belpassi, F Tarantelli, and L Storchi. [Full Parallel Implementation of an All-Electron Four-Component Dirac-Kohn-Sham Program](#). *Journal of Chemical Theory and Computation*, 10:3766–3776, 2014.
- [4] M Pastore and F De Angelis. [First-Principles Modeling of a Dye-Sensitized  \$\text{TiO}\_2/\text{IrO}\_2\$  Photoanode for Water Oxidation](#). *Journal of the American Chemical Society*, 137:5798–5809, 2015.