

Input/output CP2K/VASP/SIESTA tools

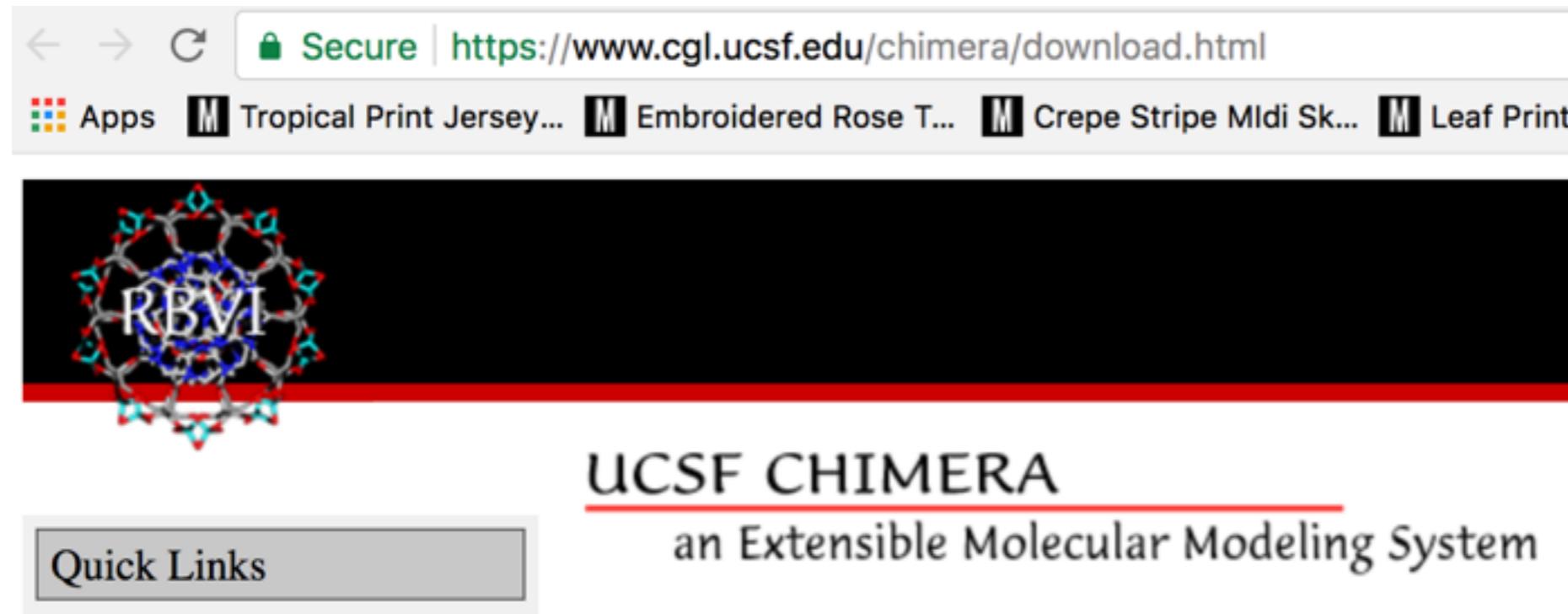
TETR - mainly an input tool (pre-processor)

- Read/write in/from different formats
- Modifications of input files
- Comparisons of geometries
- Cut out a cluster (e.g. a tip) from bulk
- prepare DOS/PDOS
- Vibrations
- Bulk => surface
- BSSE (siesta, cp2k)
- Merge geometries
- scripting

LEV00 - analyse the output files (post-processor)

- DOS/PDOS
- electron/spin density
- density algebra
- STM
- Analyse output during geometry relaxation

Tetr/Lev00 have been interfaced with CHIMERA



The screenshot shows a web browser window with the URL <https://www.cgl.ucsf.edu/chimera/download.html>. The page title is "UCSF CHIMERA" and the subtitle is "an Extensible Molecular Modeling System". On the left, there is a "Quick Links" sidebar with a logo featuring a molecular structure and the letters "RBVI". The main content area displays a molecular model of a protein or nucleic acid structure.

**Gordon Gibb, Jeremy Nowell and Iain Bethune
EPCC (Edinburgh, U.K.)**

Web access:

<https://nms.kcl.ac.uk/lev.kantorovitch/codes/lev00/index.html>