Max-Planck-Innovation

Technology Offer

BALSAC:
Build and Analyze Lattices, Surfaces, And Clusters

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PC-based software to construct lattice sections and clusters/molecules with extended graphical display and analysis options.

Version 4.10 (September 2020)

The program system **BALSAC** (**B**uild and **A**nalyze **L**attices, **S**urfaces, **A**nd **C**lusters, (C) Copyright K. Hermann, FHI 1991-2020) allows you to

interactively create, modify, display, and analyze complex crystals, single crystal surfaces, or molecules (clusters) using your personal computer or workstation. **BALSAC** can handle

- any periodic lattices, net plane stacking along any Miller index directions,
- single crystal surfaces of any reconstruction, adsorbate systems, nanotubes made of any (hkl) layers,
- crystal tips and cavities,
- molecules, atom or molecular clusters of any complexity,
- nanotubes,
- cubic nano particles

evaluate structural relationships interactively on the screen. **BALSAC** can analyze

- bonding, interatomic distances, bond angles, coordinate averages,
- packing, neighbor shells, net planes, inter-layer spacing, symmetry,
- lattice vectors, Wigner-Seitz cells, Brillouin zones, moiré vectors of interference lattices
- possible surface structures guiding experimental structure determination.

prepare figures of crystals, surfaces, and molecules, including

- opaque atom balls with various shadings, bond sticks,
- perspective views, 3-D stereo views for optical or red/blue filter glasses,
- bitmap file output of graphics windows for publications and presentations (MS Powerpoint),
- PostScript file output for publication quality prints on PostScript gray scale or color printers.

Hardware / Software Requirements

Version 4.10 for Microsoft Windows PCs with

- at least 2 GB memory
- at least 100 MB disk storage (30 MB for the installation)
- MS Windows operating system XP (SP3) and higher (32bit)

Version 2.16 for Unix / Linux workstations and Macintosh PCs with

NOTE: This version is **obsolete** and is not distributed any longer!

- (optional) ASCII text editor, e. g. vim (https://www.vim.org/), MSWord, for input/output file handling,
- (optional) PostScript viewer/printer utility, e. g. ghostview (http://pages.cs.wisc.edu/~ghost/) for graphical structure output,

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- (optional) BALSAC (http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/balpam.html) software for graphical analysis of molecular structure output.

If you are in doubt whether your hardware meets the above specifications do not hesitate to contact the author before you order.

The MS Windows version 4.10 of Balsac has been completely re-developed to run as an intrinsic MS Windows application where the present version offers as new and advanced features in particular

- **intuitive Windows handling** of most Balsac settings,
- **bitmap output** of graphics windows for MS Powerpoint and other applications,
- **extended graphical analysis** of lattice sections and clusters
- **construction of nanotubes** of most general lattice netplanes
- **new interactive help** using the html-based help engine available for Windows 7 and later

For technical and scientifical questions, please contact the author

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For further information please visit also the authors website:

http://www.fhi-berlin.mpg.de/KHsoftware/Balsac/index.html

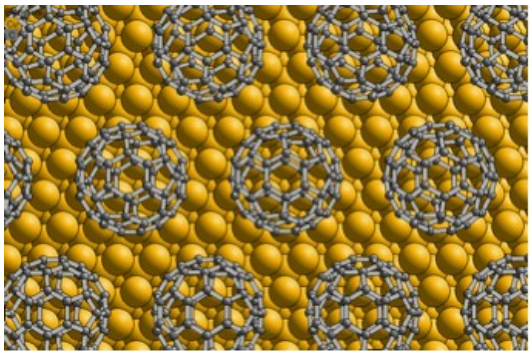
Price list for MS Windows version 4.10 of BALSAC (Validity: September 2020)

The **BALSAC** software is **copyright protected** ((C) K. Hermann, FHI 1991-2020).

Licence types (1.)	**Academic Institutions (2.)**	**Industry**
Single-user	100,- EUR	500,- EUR
Campus-licence	500,- EUR	2.500,- EUR

(Prices do not include value added tax)

1. PCR-licences are available as electronic installation packages for download - documentation via online help manual.
2. Academic institutions are universities, non-profit research laboratories, and schools.



BALSAC 4.10 example output:
Simulated structure of the Cu(111)+(4x4)-C60 adsorbate system. The C60 Buckminster balls (carbon centers are shown as small gray balls) are adsorbed with their hexagonal faces over fcc hollow sites of the Cu(111) surface (copper centers are shown as bronze colored balls).