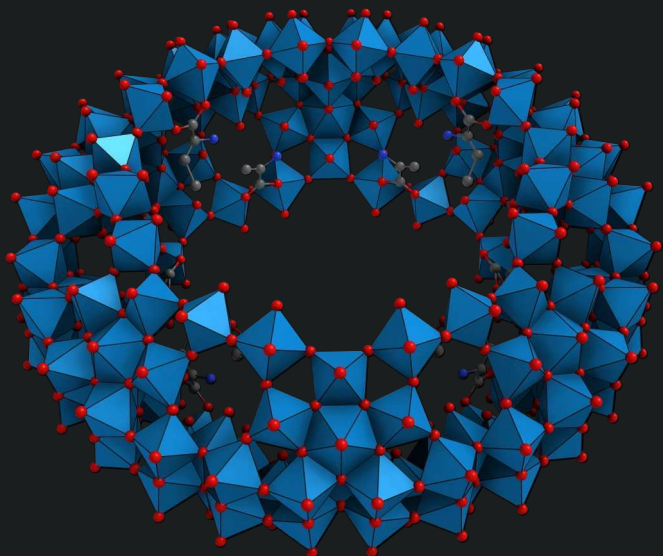


CRYSTALLOGRAPHY • QUANTUM CHEMISTRY

shapeXT

3D Structure Visualization & Interactive Analysis



High-Performance Rendering of Massive Structures

Direct Import of CIF, SHELX, DIAMOND, CUBE, XYZ

High-Res Export of 2D, Image Sequences, 3D Models

Native 64-Bit for Windows, macOS, Linux

LAUNCHING OCTOBER 2026

FREE TRIAL COMING SOON

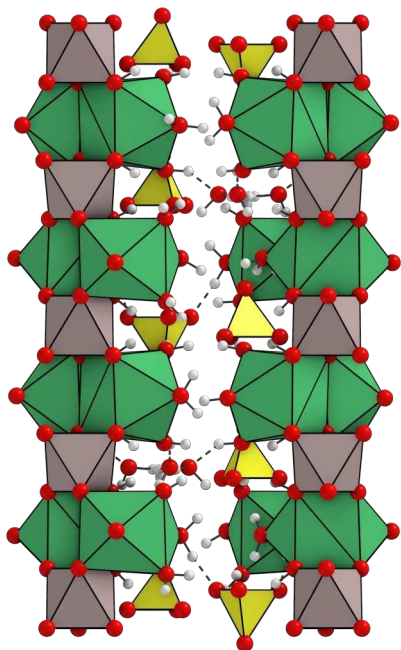
**30% EARLY BIRD DISCOUNT
UNTIL DEC 31, 2026**

www.shapeXT.com

CRYSTALLOGRAPHY & STRUCTURE MODELING

Interactive Crystal Engineering and Seamless Data Migration

- **Structure Growth & Supercells:** Multithreaded bond determination, cell filling, and supercell construction optimized for large unit cells and complex frameworks.
- **File Formats & COD Integration:** Native import for SHELX (.ins, .res), CIF, DIAMOND (.diamdoc, .dsf), and reliable COD ID structure retrieval via a dedicated backup server.
- **Wyckoff Positions & Site Occupancy:** Automatic determination of Wyckoff positions with support for mixed-occupancy sites (SOF).
- **Thermal Ellipsoids (ADPs):** Accurate representation of anisotropic displacement parameters with customizable styles, octant display, and principal axes.
- **Interactive Structure Editing:** Direct site manipulation, atom insertion/removal, and symmetry propagation across all 230 space groups.



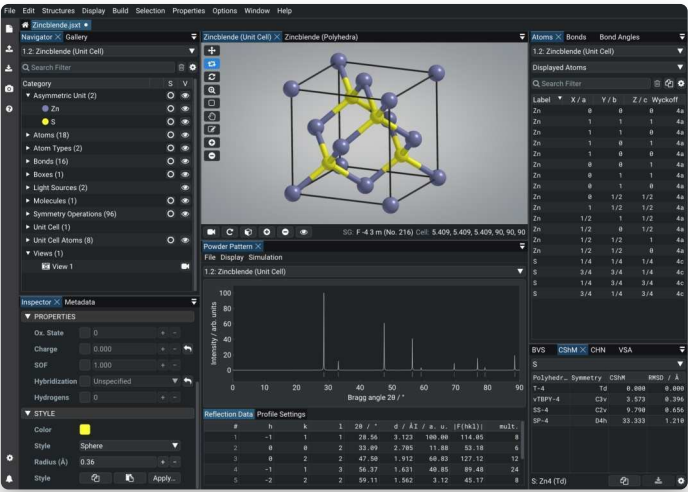
Ettringite: Polyhedral connectivity and hydrogen-bonding channels.

DIFFRACTION & PROPERTY ANALYSIS

Real-Time Physical Insight Directly from the 3D Model

- **Live Powder Diffraction (PXRD):** Real-time simulation of diffraction patterns and reflection data with dynamic updates during structure editing.
- **Quantitative Geometry & BVS:** Integrated calculation of bond valence sums (BVS), continuous shape measures (CShM), and visible solid angle (VSA) for coordination spheres.
- **Void Space & Frameworks:** Multithreaded computation of solvent-accessible pore volumes, contact surfaces, and van der Waals hulls.
- **Smart PNGs & FAIR Data:** Open JSON/UBJSON-based file architecture and image export with embedded structural data for instant drag-and-drop reload.
- **Polyhedra & Voronoi Analysis:** Construction of coordination and Voronoi polyhedra with bond-valence-assisted connectivity.

PXRD • CHN • BVS • CShM • VSA • QEq • Dipole Moment • Inertia Tensor
Voronoi Polyhedra • Contact Surface • Void Space • Promolecule Electron Density

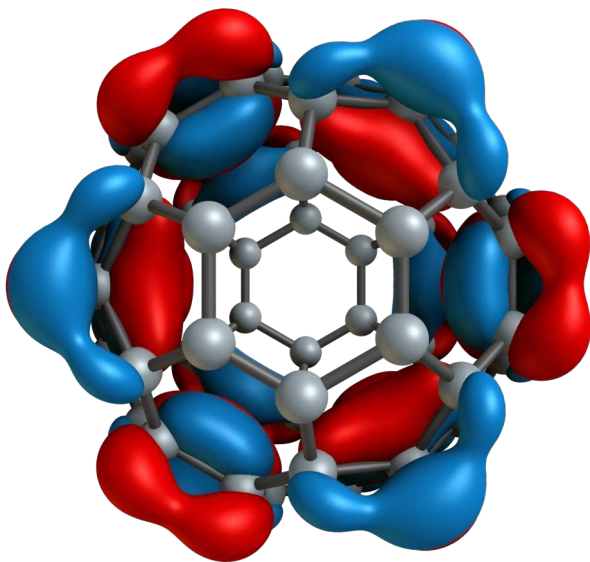


The unified shapeXT workspace with powder diffraction (PXRD).

VOLUMETRIC DATA & QUANTUM CHEMISTRY

Real-Time Orbital Rendering and Electronic Property Evaluation

- **Quantum Chemistry Formats:** Native import of Gaussian Cube (.cube), ORCA binary plot files (.plt, .3d), Turbomole (coord), and periodic VASP datasets.
- **GPU-Accelerated Isosurfaces:** Real-time isosurface calculation (marching cubes) for molecular orbitals and electron densities with live updates to isovalues, phase colors, and surface transparency.
- **Electronic Properties & Charges:** Rapid calculation of atomic partial charges (QEq-H, QEq), dipole moments, and promolecule electron densities for extended frameworks.
- **Visible Solid Angle (VSA) & Cavities:** Multithreaded ray-casting evaluation of coordination spheres, solvent-accessible contact surfaces, and framework void space.
- **Inertia Tensors & Principal Axes:** Rigorous calculation and 3D visualization of molecular inertia tensors, principal axis systems, and center-of-mass alignment.

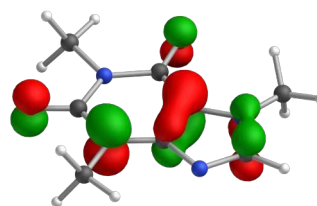


C₆₀ LUMO: Real-time isosurface generation via GPU compute shaders.

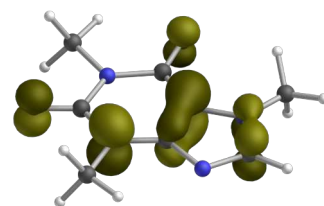
PUBLICATION WORKFLOW & EXPORT

Integrated Tools for Manuscripts, Presentations, and Supplementary Data

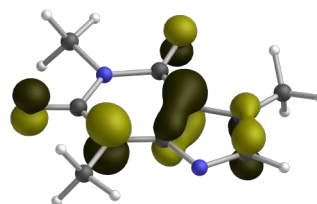
- **Scientific Annotations & Teaching:** Property vector arrows (dipole moments, magnetic anisotropy), custom labels, and on-screen drawing tools for lectures, discussions, and presentations.
- **Tabular Data & LaTeX Export:** Export atomic coordinates, bond lengths, and bond angles directly into formatted LaTeX, CSV, and plain text tables.
- **Instant Hydrogen Toggle:** Toggle hydrogen atoms and associated bonds instantly with a single keypress. Clean up figures without modifying underlying structures and datasets.
- **3D Model & Presentation Export:** Export structures to OBJ, STL, PLY, glTF/GLB, and USD for PowerPoint, Keynote, Blender, interactive web viewers, and 3D printing.
- **Accessible Figures & Color Management:** Real-time color vision deficiency (CVD) simulation, gamma correction, and modern tone mapping for publication-grade figures.



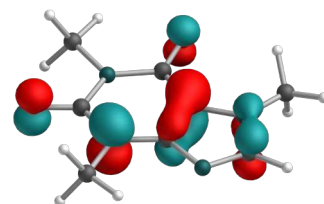
Standard Vision



Deuteranopia



Protanopia



Tritanopia

Caffeine HOMO: Color vision deficiency simulation for accessible publishing.

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Campus License	∞	2.900 € 2.030 €	5.400 € 3.780 €	7.500 € 5.250 €
– Commercial / Industry –				
Single User	1	700 € 490 €	1.300 € 910 €	1.800 € 1.260 €
Team	≤ 10	1.500 € 1.050 €	2.800 € 1.960 €	3.900 € 2.730 €
Site License	≤ 50	2.900 € 2.030 €	5.400 € 3.780 €	7.500 € 5.250 €
Enterprise	∞	5.800 € 4.060 €	10.800 € 7.560 €	15.000 € 10.500 €

30% Early Bird discount until December 31, 2026. All prices exclude VAT.



LAUNCHING OCTOBER 2026

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