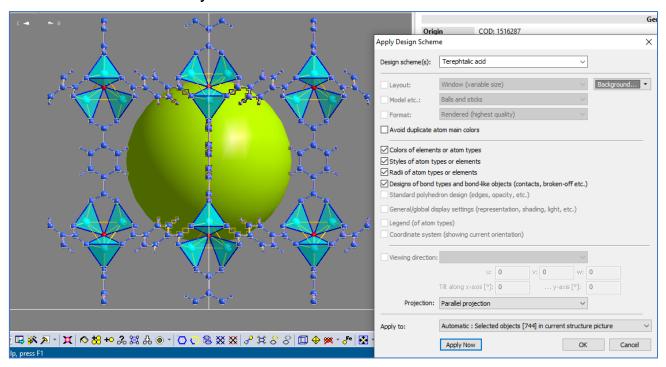


Crystal and Molecular Structure Visualization



## **New Version 5.1**

The **latest version 5.1 of Diamond** offers several new commands and functional enhancements that are especially useful when designing building units like organic linkers in Metal Organic Frameworks (MOF).

A **new Diamond version 5.2** will offer new and enhanced functions for working with **H-bonds and non-bonding contacts**:

Outstanding features introduced in version 5 are:

- ✓ The Exploration View, which enables to study (strong) bonds as well as H-bonds and non-bonding contacts when checking for neighbouring atoms and molecules in an interactive way.
- Commands Take Picture and Continue With New Picture for an improved workflow when creating multiple pictures for a structure data set.
- ✓ More Pictures docking window and Caption Bar giving a simplified overview of structure pictures.
- ✓ A newer version of Crystallography Open Database (COD; www.crystallography.net).

More outstanding functions:

- ✓ Import with automatic format recognition
- ✓ Build up structure pictures automatically or manually
- ✓ Schemes (style sheets) for building and design
- ✓ Structure type database
- ✓ Ellipsoids, disorder, mixed sites
- ✓ Molecules, packing diagrams
- ✓ Polymers and molecule clusters
- ✓ Fragmentated and broken-off bonds
- ✓ H-bonds and non-bonding contacts
- ✓ Preview of neighbouring atoms and -molecules
- ✓ Atomic environments from Dirichlet domains
- ✓ Coordination and Voronoi polyhedra
- ✓ Atom vectors, labels, and free text
- ✓ Reflection parameters and diffracion diagrams
- ✓ Distances, angles, and torsion angles
- √ hkl- and L.S.-planes and lines
- ✓ 3D export to POV-Ray, OBJ, and STL
- ✓ Video sequences and animations

Diamond version 5.1 has been released in October 2024. Version 5.2 is scheduled for the second quarter of 2025.

The update from Diamond version 4 to version 5 is free-of-charge.

https://www.crystalimpact.de/diamond/Default.htm

Price* for new License	academic	regular
Semiannual license (6 months)	162,50€	325 €
Annual license (12 months)	325 €	650 €
Single license (permanent)	649 €	1.298 €
Site license (permanent)	1.298 €	2.596 €
Campus license (permanent)	2.596 €	5.192 €

<sup>\*</sup> Prices do not include taxes which may be due.



H. Putz & K. Brandenburg GbR Kreuzherrenstr. 102 D-53227 Bonn Tel.: +49 (228) 981 36 43 Fax: +49 (228) 981 36 44 E-Mail: info@crystalimpact.de https://www.crystalimpact.de