

## ODYSSEY Molecular Explorer

| Platforms                                      |                                    | Molecular Dynamics                           |                          |
|--|------------------------------------|--|--------------------------|
| Windows  | 10, 8, 7, or Vista                 | Start Interactive Simulation                 | Single-Click             |
| macOS / OS X                                   | 10.12, 10.11, 10.10, 10.9, or 10.8 | Recommended Max. Number of Atoms             | ~1,000                   |
| Content  |                                    | Translational and Rotational Motion          | Always                   |
| Built-In Models (Molecules, Bulk Samples)      | > 3,000                            | Intramolecular Vibrational Motion            | Yes (Unless Constrained) |
| Built-In Molecular Labs                        | > 200                              | Periodic Boundaries (for Condensed Phases)   | ✓                        |
| Applied Chemistry Topics                       | > 100                              | Minimize Energy (Molecular Mechanics)        | Single-Click             |
| Models in Molecular Stockroom                  | > 1,000                            | Electron Distribution                        |                          |
| New User Tutorials (for Operating Program)     | 14                                 | Calculate (from Quantum Mechanics)           | Single-Click             |
| Content Search Engine                          | ✓                                  | Max. Number of Atoms                         | 30                       |
| Hyperlinks to Wikipedia                        | ✓                                  | Electron Density Isosurfaces                 | ✓                        |
| Periodic Table of the Elements                 | ✓                                  | Polarity Maps (Electrostatic Potential Maps) | ✓                        |
| Lists of Misconceptions                        | <i>Instructor's Ed. Only</i>       | Atomic Orbitals                              | Selected Examples        |
| Comments                                       | All Labs                           | Molecular Orbitals                           | Selected Examples        |
| Assessment Questions                           | ~1,200                             | Electrostatic Potentials, Spin Densities     | Selected Examples        |
| Answer Key                                     | <i>Instructor's Ed. Only</i>       | Chemical Reactions                           |                          |
| Add Model Snapshots to Answers                 | ✓                                  | Reaction Dynamics at Set Temperature         | Selected Examples        |
| Annotation of Pages                            | ✓                                  | Dynamic Equilibria                           | Selected Examples        |
| Customize Questions                            | <i>Instructor's Ed. Only</i>       | Examine Reaction Profiles                    | Selected Examples        |
| Authoring Capability                           | <i>Instructor's Ed. Only</i>       | Building New Models                          |                          |
| 3D Visualization                               |                                    | New User Tutorials (for Building Models)     | 25                       |
| Styles (Wire, Ball&Spoke, Space Filling, etc.) | 5                                  | Max. Number of Atoms, Crystal Builder        | 1,500                    |
| Use Multiple Styles in Same Model              | ✓                                  | Max. Number of Atoms, General                | 9,999 (per Atom Type)    |
| Show Two Models Side-by-Side                   | ✓                                  | 3D Entry-Level Builder                       | ✓                        |
| Synchronize Side-by-Side Simulations           | ✓                                  | 3D Advanced/Inorganic Builder                | ✓                        |
| Scroll through Daisy-Chained Models            | Selected Examples                  | 3D Crystal Builder (Solids)                  | 52 Templates             |
| Show Hydrogen Bonding, Show Dipoles            | ✓                                  | 3D Disordered Phase Builder (Gases, Liquids) | ✓                        |
| Show Idealized Lone Pair Positions             | ✓                                  | 3D Peptide and Nucleotide Builders           | ✓                        |
| Show Collisions, Show Reactive Events          | ✓                                  | Chemical Validity Check                      | ✓                        |
| Show Velocity Vectors, Show Trajectories       | ✓                                  | Name Molecules (Systematic Names)            | ✓                        |
| Ribbons for Biopolymers                        | ✓                                  | Show Common Names (for Built-In Models)      | ✓                        |
| Hyperlinkable from PowerPoint                  | ✓                                  | Add Arbitrary Labels                         | ✓                        |
| Export of JPG/PNG/BMP Images                   | ✓                                  | PDB/ChemDraw/SMILES Import                   | Drag and Drop            |
| SMILES Export (EXPERT Setting)                 | ✓                                  | Analysis                                     |                          |
| Declare Custom Colors                          | ✓                                  | Measure Distances and Angles                 | ✓                        |
| Anaglyph Red-Blue Stereo                       | ✓                                  | Measure Torsion Angles                       | ✓                        |
| Changing Parameters                            |                                    | Other Property Queries                       | Many                     |
| Change Bond Lengths and Torsion Angles         | ✓                                  | Extended Property List (EXPERT Setting)      | ✓                        |
| Move Molecules Relative to Each Other          | ✓                                  | XY Plots and Histograms                      | ✓                        |
| Change Temperature and/or Cell Volume          | ✓                                  | Linear Regression                            | ✓                        |
| Change Numbers of Molecules                    | ✓                                  | Reciprocal and Logarithmic Axes              | ✓                        |
| Change Time Step (to Slow Down Motion)         | ✓                                  | Radial Distrib. Function (EXPERT Setting)    | ✓                        |