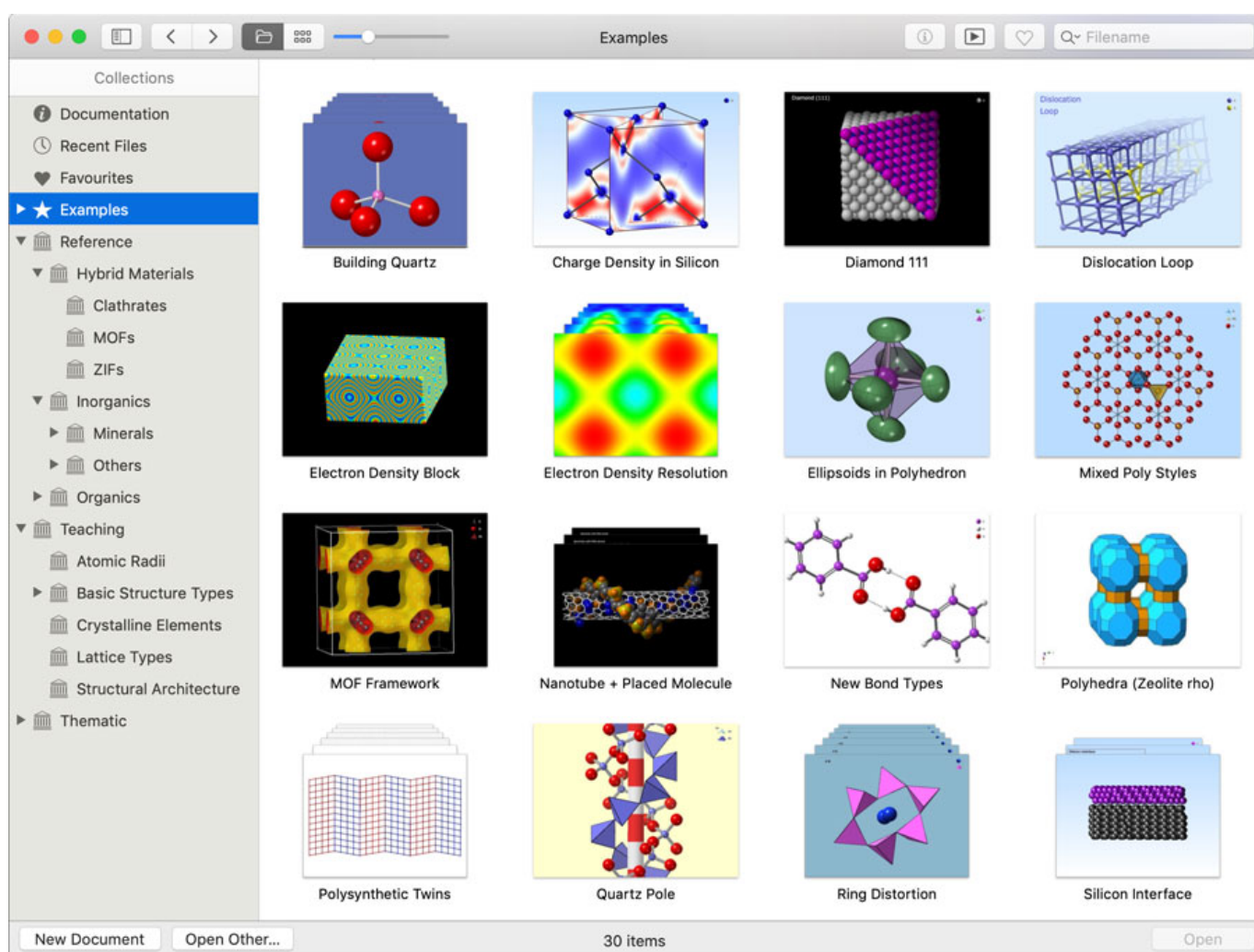[Lattice Parameter Calculation Software Free 14](#)

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XLAT (LSQ) program for the precise refinement of cell constants. ... for each phase as required (5) lattice parameter fitting and diffraction intensity calculation.. applications free software MAUD, GaussView and HyperChem which facilitate the process of ... applications are used to estimate lattice parameters in molecules. ... [13] and Cu2O [14] (b) compared with crystallography information file (CIF).. Figure 1 Shows the minimum total energy and lattice constant of the spinel ... The application of DFT to calculate the ground state properties of materials is highly .... relatively constant, the reflection with the largest Bragg angle is chosen to minimize error in the lattice parameter calculation (or perform least squares on.. http://www.ccp14.ac.uk/solution/indexing/. Here, u can find a software called "Unit Cell" which is useful for calculating lattice parameters and unit cell volume.. A new computer program, implementing nonlinear regression methods and providing the ... I~YWORDS: powder diffraction, regression diagnostics, lattice parameters, computer program. Introduction ... equation (2) above is only linear in parameters xl ... x6 ... other hand, Table 3 shows that the 7~14 reflection is a true outlier ...

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