CrystalMaker v11.5.1.300 (Win)

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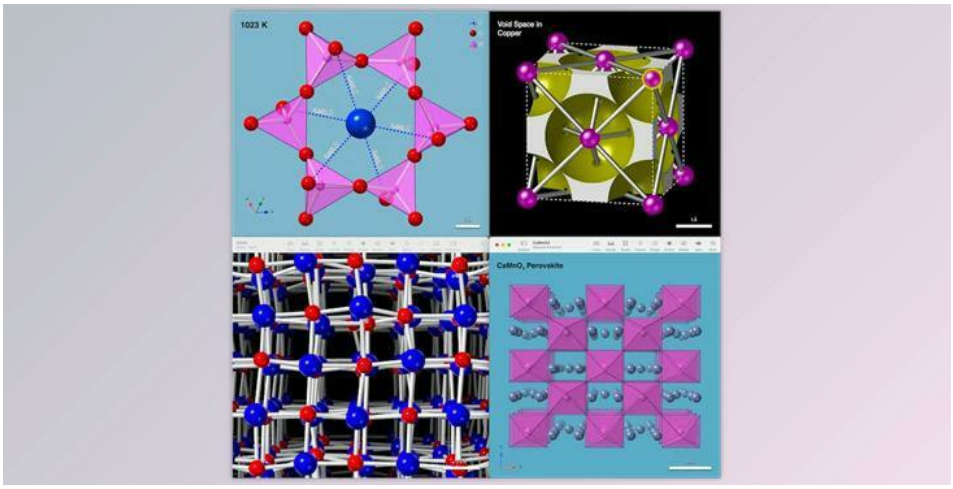

CrystalMaker 11.0.0.300 (Win):

CrystalMaker stands as the most efficient means of visualizing crystal and molecular structures. Through its interactive design, it empowers users to grasp the intricacies of complex materials, allowing them to "see the wood for the trees" and construct their visual understanding. Going beyond traditional crystallography software, CrystalMaker facilitates the creation of dynamic visualizations with rotatable animations. Its energy-modeling tools enable users to design and relax new structures, predict vibrational properties, and explore their interactions with other materials.

The culmination of a decade-long research project, CrystalMaker 11 represents a significant milestone. During this period, a Ph.D. project and a Knowledge Transfer Partnership (KTP) were sponsored, aiming to develop accessible energy modeling and lattice dynamics tools for personal computers. This aligns with the overarching goal of CrystalMaker – to provide the best visual understanding of complex structures and properties, making workstation-level tools accessible to a broader scientific computer audience, without the reliance on energy-intensive supercomputers.

CrystalMaker 11 introduces its integrated crystal-energy modeling engine, featuring a substantial library of parameterized potentials. The program employs intelligent selection criteria based on existing bonding criteria and a detailed understanding of atomic environments. Energy minimization is achieved through a novel hybrid Monte Carlo and least-squares technique, allowing for real-time relaxation, even for surfaces. This innovative approach positions CrystalMaker 11 as a powerful tool for researchers and scientists seeking advanced capabilities in structural analysis and energy modeling.

Phonons Explorer:

- CrystalMaker 11 has the capability to calculate vibrational modes, including dispersion curves and structural animations, for crystals. It visualizes lattice waves, known as "phonons," at any point in reciprocal space. Users can specify two points in reciprocal space to display corresponding dispersion curves. Clicking on a point on a dispersion curve allows the definition of a wave vector and visualization of its vibrational mode.

Simulate Temperature & Pressure:

- The "Simulate Temperature & Pressure" command enables users to simulate the effects of temperature and, optionally, pressure. CrystalMaker conducts a Monte Carlo simulation using either constant volume ("NVT") or constant pressure ("NPT") based on the specified temperature/pressure. The structure, ideally a supercell, is dynamically updated in real-time, with energy values plotted. This feature not only offers interactive visualization of structural changes but also serves as a practical tool for introducing disorder into an otherwise ideal material, creating an "amorphous" structure for subsequent modeling calculations.

Physical & Thermodynamic Properties:

- As part of its energy modeling capabilities, CrystalMaker can calculate the density of states for crystals. This information is presented as a histogram, illustrating the relative population of different vibrational frequencies. These underlying calculations are crucial for predicting various physical and thermodynamic properties, enhancing the software's utility for comprehensive material analysis.

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