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Development of Virtual Laboratory for Multifunctional Material Characterization

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ABSTRACT

The rapid advancement of material science has necessitated the development of innovative tools for material characterization. This paper discusses the creation of virtual laboratory software specifically designed for the characterization of multifunctional materials. Traditional experimental methods often pose challenges in terms of cost, time, and resource availability, whereas virtual laboratories provide a flexible and efficient alternative. Key features of the software include advanced simulation capabilities, a user-friendly interface, robust data analysis tools, and integration with experimental data. The development process involves requirement analysis, design and prototyping, implementation, testing and validation, and deployment and training. Applications of the software span across materials science, engineering, and education, offering significant benefits such as cost savings, time efficiency, enhanced research capabilities, and improved collaboration. This virtual laboratory software represents a significant step forward in material characterization, enabling researchers to conduct comprehensive and precise analyses in a simulated environment, thereby accelerating discoveries and innovations in the field. In this research, an algorithm for manual interface with theoretical data was developed to generate the properties of elements in accordance with their periodic table arrangement. The powder plot jar. was also developed for generating cif file of the functional material. Finally the efficiency performance of the developed multifunctional characterization software was tested and the results obtained is in accordance with reported literature.

Keywords: Virtual Laboratory, Functional materials Characterization, Cif file generation, Computational Modelling

1.0 INTRODUCTION

The field of material science is undergoing a transformation with the advent of virtual laboratory software. These digital platforms provide a powerful means to simulate and analyse the properties and behaviours of multifunctional materials. Multifunctional materials are those that possess multiple properties or functions, making them suitable for a wide range of applications in industries such as aerospace, automotive, and electronics **[1].** Traditional methods of characterizing these materials often involve complex, time-consuming, and costly experiments. Virtual laboratories, however, offer a cost-effective and efficient alternative, enabling researchers to conduct detailed simulations and analyses in a controlled digital environment **[2].** The traditional experimental methods for material characterization present several challenges such as: cost and resource constraints which involves a physical experiment that requires extensive resources, including materials, equipment, and labour, which can be costly and limited in availability [3], time-consuming processes where the experimental setups, execution, and analysis can take considerable time, delaying research progress and limited flexibility in which physical experiments may be constrained by environmental and logistical factors **[4],** limiting the range of conditions that can be tested, these aforementioned factors necessitate the need for virtual laboratories [5,6].

In contrast, virtual laboratories provide a solution to the aforementioned challenges by allowing researchers to perform simulations in a digital environment. This not only reduces the need for physical resources but also offers flexibility in testing various conditions and scenarios that might be difficult or impossible to achieve experimentally **[7].** The virtual laboratories reduce the need for physical resources and experimental setups, resulting in significant cost savings. Researchers can conduct extensive simulations without the expenses associated with traditional experiments. Also, Simulations can be conducted and analyzed much faster than physical experiments, accelerating the pace of research and discovery **[9].** This allows researchers to quickly iterate on their designs and hypotheses. Virtual laboratories enable researchers to test a wide range of conditions and scenarios that may be difficult or impossible to achieve experimentally. This expands the scope of research and opens up new possibilities for innovation. The digital nature of virtual laboratories makes it easy for researchers to share simulations, data, and findings with collaborators worldwide. This fosters collaboration and the exchange of ideas, leading to more comprehensive and impactful research. Virtual laboratory software for multifunctional material characterization has a wide range of applications in various fields, including materials science and engineering **[10].**

In this research, an algorithm for manual interface with theoretical data through structure tidy exe was developed to generate chemical and physical properties of elements in accordance with their periodic table arrangement. The powder plot jar. through java (TM) platform SE binary was also developed for generating cif file of the functional material finally the efficiency performance of the developed multifunctional characterization software was tested and the results obtained is in accordance with reported literature **[11,12].**

2. METHODOLOGY

2.1 Required Features for Virtual Laboratory Software

Several key features were taken into consideration for the development of *"Bee-Cube"* virtual laboratory software for multifunctional material characterization to ensure accuracy, usability, and versatility such as:

Simulation Capabilities: At the core of any virtual laboratory software are its simulation capabilities. Advanced computational models and algorithms are used to accurately simulate the physical and chemical properties of materials under various conditions. So that the simulations will replicate real-world scenarios, providing reliable data for further analysis.

User-Friendly Interface: A well-designed user interface is crucial for making the software accessible to researchers with varying levels of technical expertise. Features such as intuitive navigation, clear visualization tools, and comprehensive tutorials enhance the user experience, allowing researchers to focus on their experiments without being hindered by complex software operations.

Data Analysis Tools: Robust data analysis tools are essential for interpreting the results of simulations. The software should provide a range of analytical tools, including statistical analysis, graphical representation, and comparison with experimental data. These tools enable researchers to extract meaningful insights from their simulations and validate their findings.

Customization and Scalability: The software should be customizable to meet the specific needs of different research projects and scalable to handle complex simulations involving large datasets or high-performance computing resources. This flexibility ensures that the software can be used for a wide range of applications and research scenarios.

Integration with Experimental Data: To ensure the accuracy and reliability of simulation results, the software should be able to integrate with experimental data. This allows researchers to cross-verify their simulations with real-world data, refine their models, and improve the accuracy of their predictions.

2.2 Development Process for Virtual Laboratory Software

The development of virtual laboratory software typically follows a structured process involving several stages:

Requirement Analysis: The first step in developing virtual laboratory software is to understand the specific needs of researchers and the types of materials to be characterized. This involves close collaboration with material scientists, engineers, and other stakeholders to gather detailed requirements and define the scope of the project.

Design and Prototyping: Once the requirements are clearly defined, the next step is to create initial designs and prototypes of the software. This stage focuses on developing the core functionalities and user interface design. Feedback from potential users is crucial at this stage to refine the design and ensure that the software meets their needs.

Implementation: During the implementation phase, the software is developed using appropriate programming languages and tools. This involves coding the simulation algorithms, developing the user interface, and integrating data analysis tools. The implementation phase requires careful attention to detail to ensure that the software functions as intended and meets the required performance standards.

Testing and Validation: Rigorous testing is conducted to ensure that the software functions correctly and produces accurate results. This includes unit testing, integration testing, and validation against experimental data. Testing and validation are critical to identify and fix any bugs or issues and to ensure the reliability and accuracy of the software.

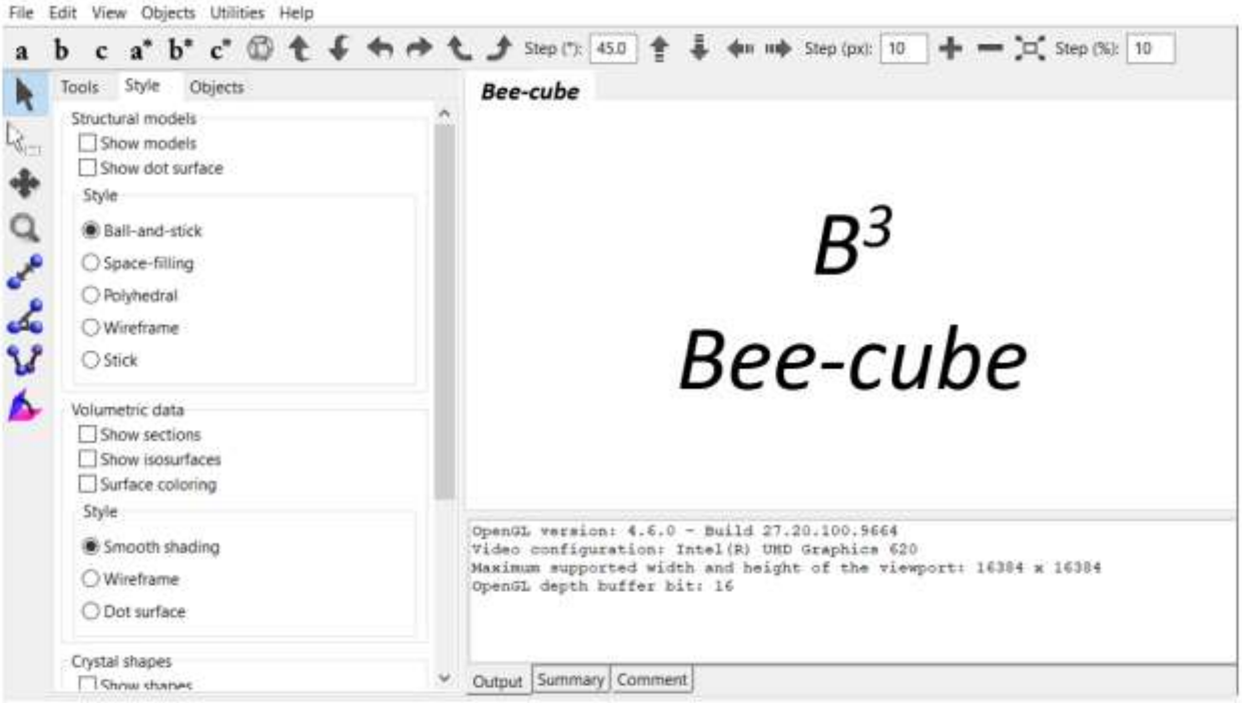
Deployment and Training: Once the software is fully developed and tested, it is deployed for use by researchers. Training sessions and user manuals are provided to help users get acquainted with the software and its features. Ongoing support and training are essential to ensure that users can effectively utilize the software for their research.

Maintenance and Updates: Ongoing maintenance and updates are necessary to keep the software up-to-date with the latest scientific advancements and to address any issues that arise. Regular updates ensure that the software remains relevant and continues to meet the needs of researchers.

3.0 RESULT AND DISCUSSION

3.1 Designed User-Friendly Interface

The **Figure 1**, below shows the user friendly designed in this research, the logo of the software was derived from the first latter each of the researchers name i.e., **B^3 = Bilkisu, Babangida, Bashir.** The features of the software were designed to be use in an easier way to the beginner, it is just occupies 12mb of the computer storge, it can also be deposited on the internet for easy access. Bee-cube software can perform a multifunctional material characterization such as: X-ray diffraction (XRD) for that determine structural formation of the material, Photoluminescence (PL) spectroscopy & ultraviolet visible (U.V vis) spectroscopy both used to determine the optical properties of the functional material, Thermo-Gravimetric Analysis (TGA) for identifying the thermal stability of the functional material, Impedance spectroscopy (IS) for finding the storage capacity in super conducting material and many more by the use of the generated crystallographic information file (CIF.FILE). **Figures 2-7**, shows the step-by-step example on how the XRD pattern for Copper Oxide (Cu_2O) nanomaterial was obtained, and the result tallied with international crystallographic data base (ICDB) with the deposited No. 1291512, the structural pattern of Cu_2O was also found to be in good agreement with the reported literature **[13].**



Structural models

☐ Show models

☐ Show dot surface

Style

● Ball-and-stick

○ Space-filling

○ Polyhedral

○ Wireframe

○ Stick

Volumetric data

☐ Show sections

☐ Show isosurfaces

☐ Surface coloring

Style

● Smooth shading

○ Wireframe

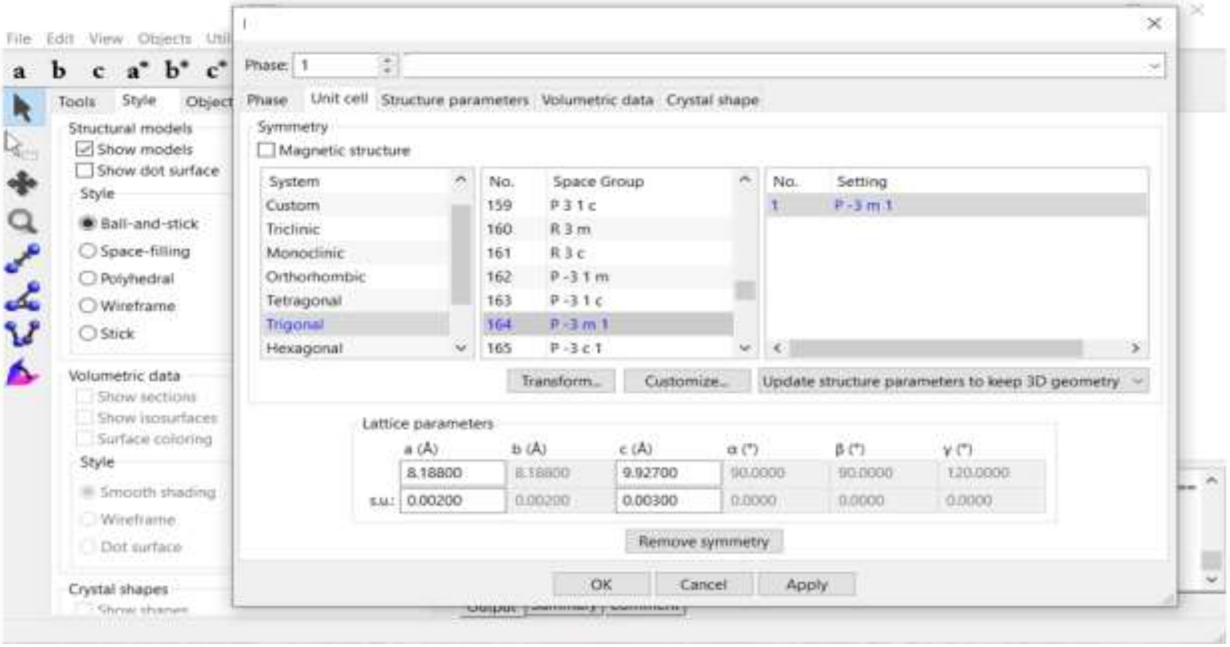
○ Dot surface

Crystal shapes

☐ Show shapes

```
OpenGL version: 4.6.0 - Build 27.20.100.9664
Video configuration: Intel(R) UHD Graphics 620
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16
```

Figure 1: User-Friendly Interface for Bee-cube software



Phase: 1

Symmetry

☐ Magnetic structure

System
Custom
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal
Hexagonal

No.	Space Group
159	P 3 1 c
160	R 3 m
161	R 3 c
162	P -3 1 m
163	P -3 1 c
164	P -3 m 1
165	P -3 c 1

No.	Setting
1	P -3 m 1

Lattice parameters

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
	8.18800	8.18800	9.92700	90.0000	90.0000	120.0000
s.u.:	0.00200	0.00200	0.00300	0.0000	0.0000	0.0000

Structural models

☑ Show models

☐ Show dot surface

Style

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○ Wireframe

○ Stick

Volumetric data

☐ Show sections

☐ Show isosurfaces

☐ Surface coloring

Style

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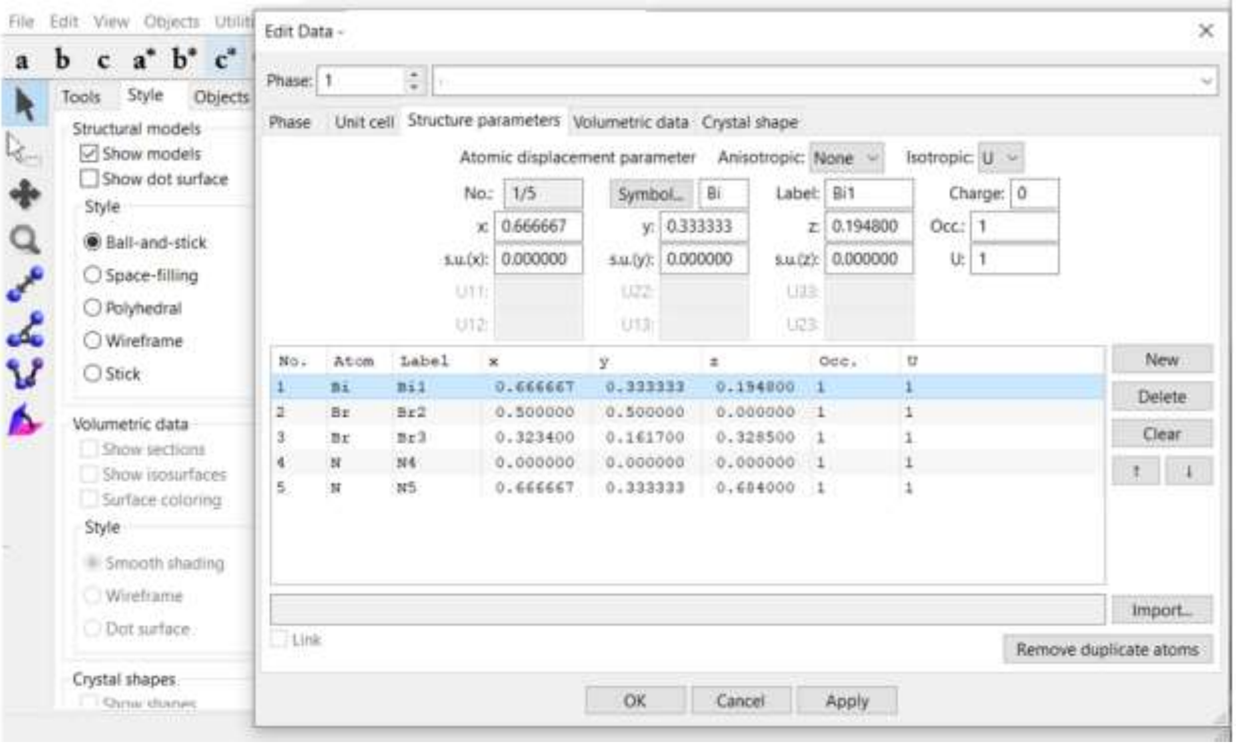
○ Wireframe

○ Dot surface

Crystal shapes

☐ Show shapes

Figure 2: Crystal system page of Bee-cube software



☑ Show models
☐ Show dot surface
● Ball-and-stick
○ Space-filling
○ Polyhedral
○ Wireframe
○ Stick
☐ Show sections
☐ Show isosurfaces
☐ Surface coloring
● Smooth shading
○ Wireframe
○ Dot surface
☐ Show shapes

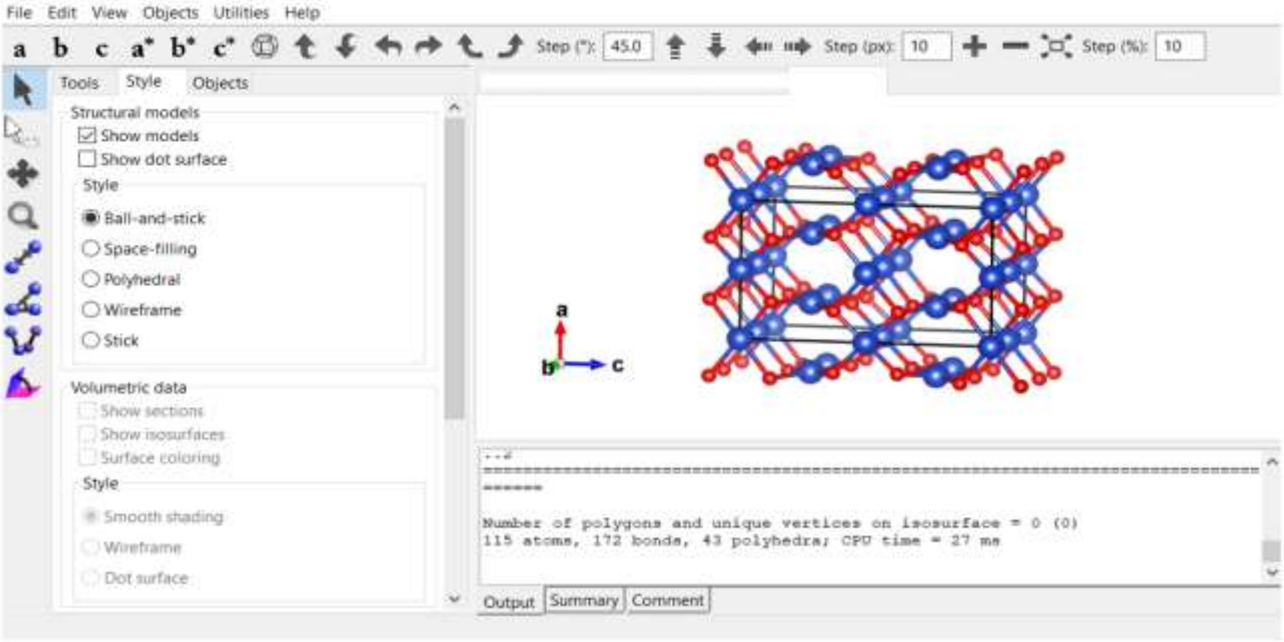
Phase: 1

Atomic displacement parameter Anisotropic: None Isotropic: U

No.: 1/5 Symbol... Bi Label: Bi1 Charge: 0
x: 0.666667 y: 0.333333 z: 0.194800 Occ.: 1
s.u.(x): 0.000000 s.u.(y): 0.000000 s.u.(z): 0.000000 U: 1

No.	Atom	Label	x	y	z	Occ.	U
1	Bi	Bi1	0.666667	0.333333	0.194800	1	1
2	Br	Br2	0.500000	0.500000	0.000000	1	1
3	Br	Br3	0.323400	0.161700	0.328500	1	1
4	N	N4	0.000000	0.000000	0.000000	1	1
5	N	N5	0.666667	0.333333	0.684000	1	1

Figure 3: Structural parameter page of Bee-cube software



Step (°): 45.0 Step (px): 10 Step (%): 10

☑ Show models
☐ Show dot surface
● Ball-and-stick
○ Space-filling
○ Polyhedral
○ Wireframe
○ Stick
☐ Show sections
☐ Show isosurfaces
☐ Surface coloring
● Smooth shading
○ Wireframe
○ Dot surface

```
==================================================================================
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Number of polygons and unique vertices on isosurface = 0 (0)
115 atoms, 172 bonds, 43 polyhedra; CPU time = 27 ms
```
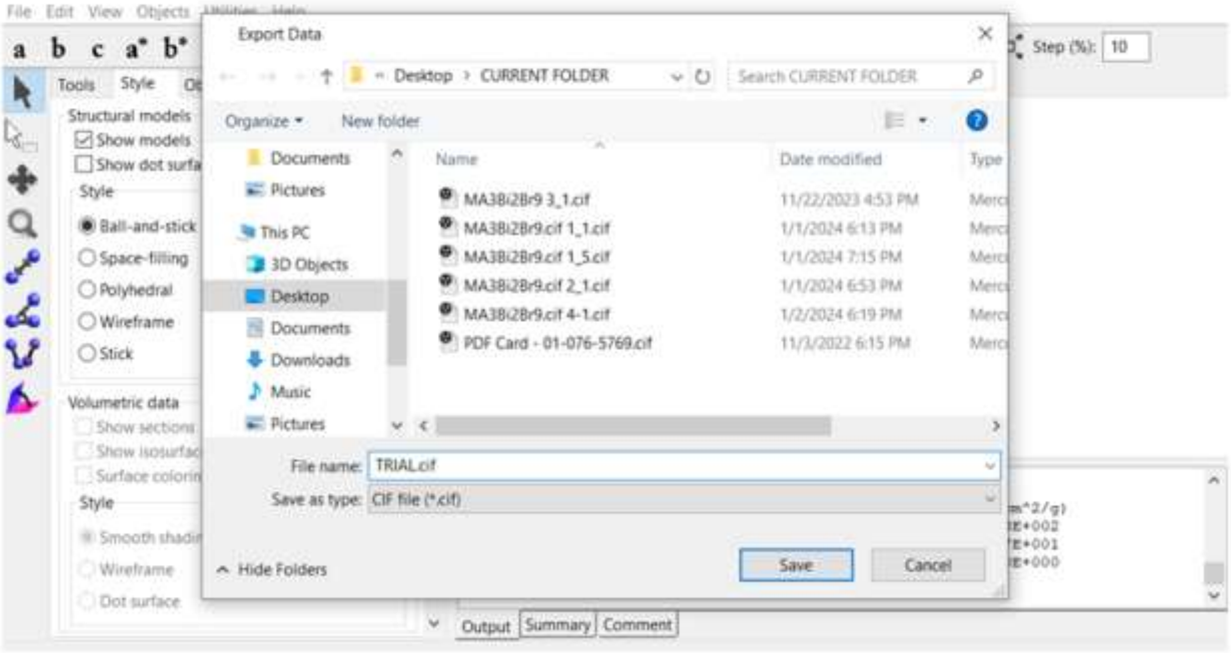

Figure 4: Structural patter page of Bee-cube software

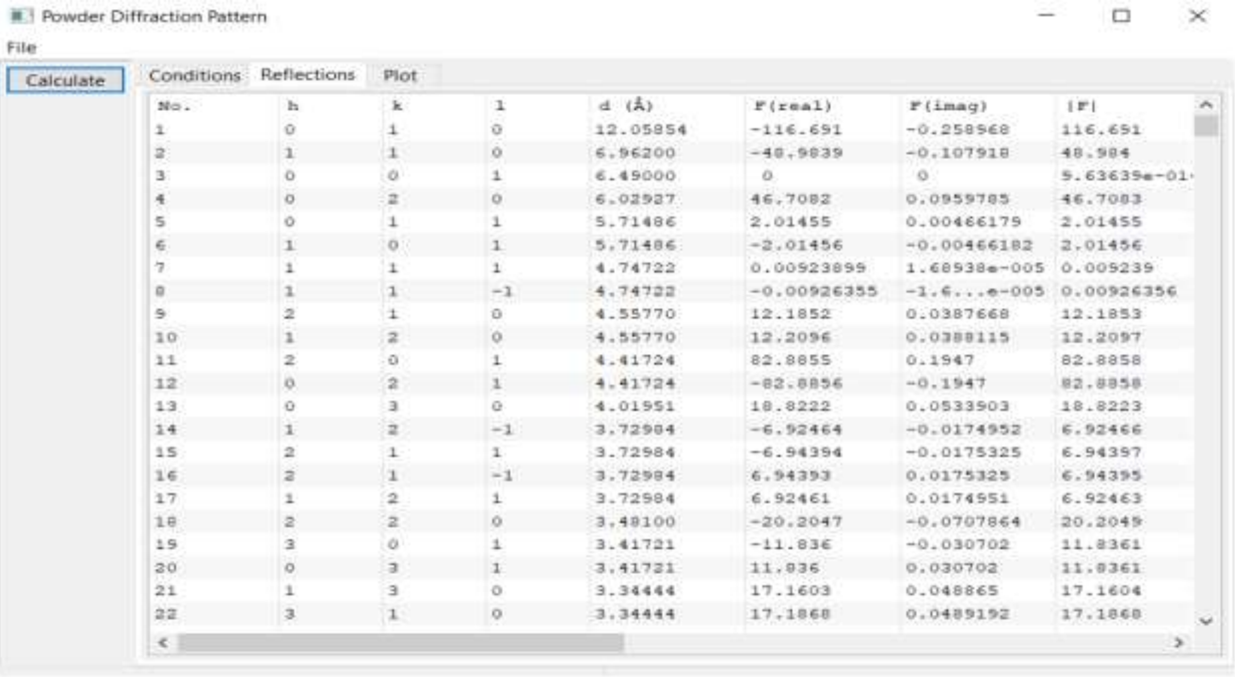


Name	Date modified	Type
MA3Bi2Br9 3_1.cif	11/22/2023 4:53 PM	Merc
MA3Bi2Br9.cif 1_1.cif	1/1/2024 6:13 PM	Merc
MA3Bi2Br9.cif 1_5.cif	1/1/2024 7:15 PM	Merc
MA3Bi2Br9.cif 2_1.cif	1/1/2024 6:53 PM	Merc
MA3Bi2Br9.cif 4-1.cif	1/2/2024 6:19 PM	Merc
PDF Card - 01-076-5769.cif	11/3/2022 6:15 PM	Merc

File name: TRIAL.cif

Save as type: CIF file (*.cif)

Figure 5: Cif-file page of Bee-cube software



No.	h	k	l	d (Å)	F(real)	F(imag)	|F|
1	0	1	0	12.05854	-116.691	-0.258968	116.691
2	1	1	0	6.96200	-48.9839	-0.107918	48.984
3	0	0	1	6.49000	0	0	5.63635e-01
4	0	2	0	6.02927	46.7082	0.0959785	46.7083
5	0	1	1	5.71486	2.01455	0.00466179	2.01455
6	1	0	1	5.71486	-2.01456	-0.00466182	2.01456
7	1	1	1	4.74722	0.00923899	1.68938e-005	0.009239
8	1	1	-1	4.74722	-0.00926355	-1.6...e-005	0.00926356
9	2	1	0	4.55770	12.1852	0.0387668	12.1853
10	1	2	0	4.55770	12.2096	0.0388115	12.2097
11	2	0	1	4.41724	82.8855	0.1947	82.8858
12	0	2	1	4.41724	-82.8856	-0.1947	82.8858
13	0	3	0	4.01951	18.8222	0.0533903	18.8223
14	1	2	-1	3.72984	-6.92464	-0.0174952	6.92466
15	2	1	1	3.72984	-6.94394	-0.0175325	6.94397
16	2	1	-1	3.72984	6.94393	0.0175325	6.94395
17	1	2	1	3.72984	6.92461	0.0174951	6.92463
18	2	2	0	3.48100	-20.2047	-0.0707864	20.2049
19	3	0	1	3.41721	-11.836	-0.030702	11.8361
20	0	3	1	3.41721	11.836	0.030702	11.8361
21	1	3	0	3.34444	17.1603	0.048865	17.1604
22	3	1	0	3.34444	17.1868	0.0489192	17.1868

Figure 6: Calculated XRD raw data from Bee-cube software

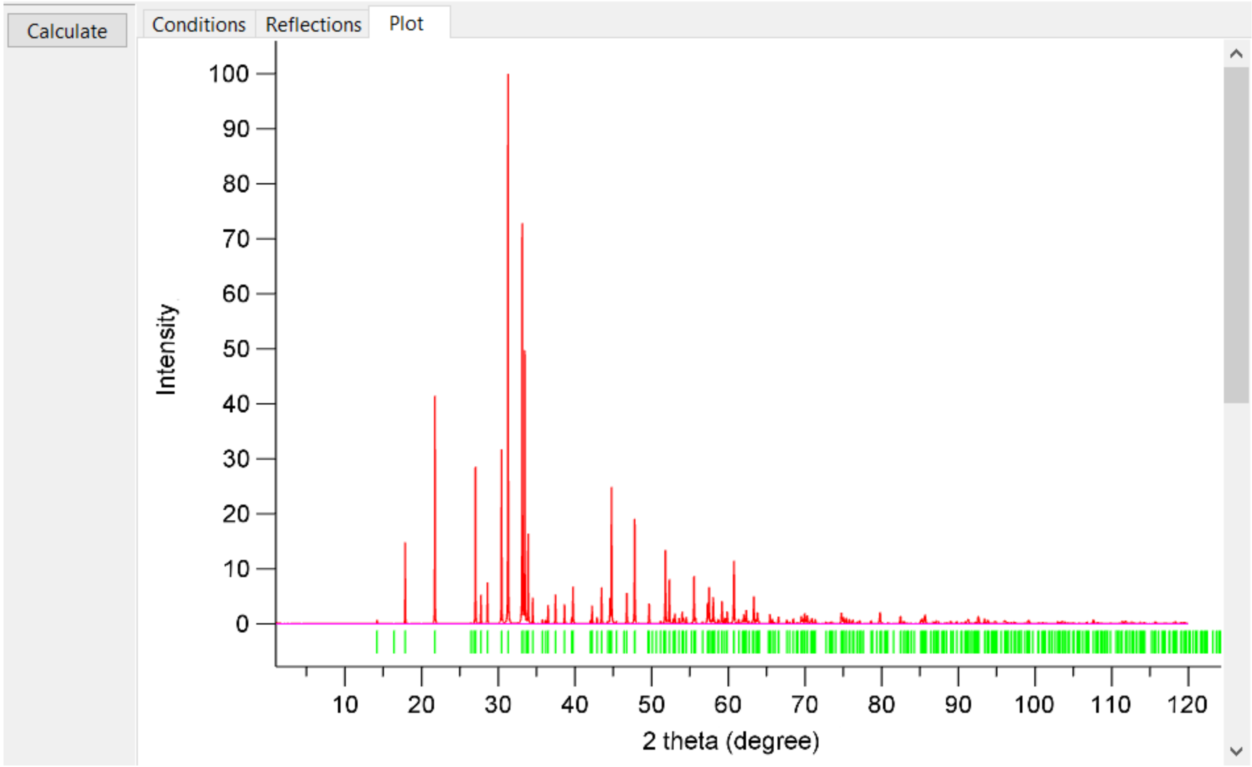


Figure 7: XRD pattern from Bee-cube software

4.0 CONCLUSION

The development of virtual laboratory software for multifunctional material characterization represents a significant advancement in material science research. By providing a flexible, cost-effective, and powerful tool for simulating and analysing materials, virtual laboratories have the potential to accelerate discoveries, improve material performance, and drive innovation across various industries. As technology continues to evolve, the capabilities of virtual laboratory software will only expand, offering even greater possibilities for researchers and engineers. This transformative tool not only enhances our understanding of multifunctional materials but also paves the way for the development of new materials with unprecedented properties and applications.

Bee-cube software was tested to be able to perform a multifunctional material characterization such as: XRD for that determine structural formation of the material, PL spectroscopy & U.V vis spectroscopy both used to determine the optical properties of the functional material, Thermo- TGA for identifying the thermal stability of the functional material, Impedance spectroscopy for finding the storage capacity in super conducting material and many more by the use of the generated Cif. File.

The step-by-step example on how the XRD pattern for Copper Oxide (Cu_2O) nanomaterial was obtained, and the result tallied with international crystallographic data base (ICDB) with the deposited No. 1291512, the structural pattern of Cu_2O was also found to be in good agreement with the reported literature

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