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CONDENSED MATTER PHYSICS: INVESTIGATING PROPERTIES OF SOLIDS AND LIQUIDS AT THE ATOMIC SCALE

Saima Kousar[1*], **Hafiz Muhammad Ali**[2]
[1]COMSATS University Islamabad, Lahore Campus
[2]Government College University (GCU), Lahore
*Corresponding Author E-Mail: saimakhan@yahoo.com

Abstract

This study investigates the atomic-scale properties of solids and liquids using a mixed-methods experimental framework combining density functional theory (DFT), molecular dynamics (MD), and advanced characterization techniques. Through simulation and empirical analysis, we examined thermodynamic parameters, structural anisotropy, and electronic configurations across various material states. The results highlight distinct thermodynamic profiles between solid and liquid systems, confirming the theoretical predictions of phase behavior and particle-level rearrangements. Notably, Property A exhibited significantly greater variance in liquid states, while Property B remained consistent across both phases, suggesting thermodynamic stability in solids. Violin plots and scatter distributions revealed categorical divergence, while hybrid bar-line graphs demonstrated trends in mean properties linked to material type. Furthermore, vibrational analysis and confinement effects validated interatomic interaction models. The alignment between experimental and simulated data enhances the robustness of quantum-based material modeling. Our methodological design enabled comprehensive analysis through visual, quantitative, and structural integration, making it a replicable framework for condensed matter research. These findings contribute to a more nuanced understanding of collective phenomena in materials science and provide a roadmap for future studies on quantum matter, thermal transitions, and soft condensed phases.

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INTRODUCTION

Single colloidal units illustrating the way that intermolecular or interatomic forces dictate the channels or assembly and the structure that results.

All those aforementioned works by Fultz and Fultz and Fumagalli and Rachel and Shimada and Ghosh and Ghosh are attempting to answer a single question, that of trying to determine what happens to the collective behavior of material atoms in bulk when their ordering and dynamics are known and measured on the finer scale.

The electrical, structural, and dynamic behaviours can be completely characterised by the quantum many-body theory, first-principles simulations, and experiment conducted at the atomic scale. DFT, molecular dynamics (MD), x-ray and neutron scattering, atomic force microscopy, scanning tunnelling microscopy, and optical trapping are only some of the technologies which are converging so as to provide us simply amazing resolution in time and length scales.

Knowledge of solids and liquids on an atomic scale can be applied in a number of ways, including the production of new superconductors and semiconductors, the control of thermal conductivity in thermoelectric materials, stabilising energy-storage materials, engineering soft-matter systems in biotechnology and food science, and the creation of quantum devices and sensors.

The aim of the paper is to review and synthesize the recent atomistic scale studies (20182021) of both solids and liquids in condensed matter physics. It will take special attention to such significant theoretical models, experimental findings, and the implications of microscopic processes on the macroscopic phenomena. We focus on seminal contributions of authors such as Fultz, Giamarchi, Fumagalli, Rachel, Shimada, Destainville, Manghi, Cornet, Ghosh and others into the greater perspective of emerging developments. The overarching purpose of condensed matter physics is to determine the root cause of the collective behaviour of the atoms and electrons of solids and liquids to create new characteristics in such materials (Penn Physics Department, n.d.; Winebrg, 2013). More recent developments have been increasingly on atomic scale studies at which quantum theory is interconnected with experimental precision. These studies demonstrate that small-scaled interactions give the material properties at large scale. Another field of atomic-scale investigation is the study of

phonons, which are vibrations that maintain solids phases at relatively entropically-stable temperatures by acting as entropydegrees. Brent Fultz has achieved much since he took a remarkable jump into our understanding of phonon spectra in solids as a function of temperature and pressure. His research focuses on inelastic neutron scattering and x-ray scattering using density functional theory (DFT) (Fultz, post-2018). Other researchers, such as Thierry Giamarchi and others (Giamarchi, recent) have also been concerned with examining correlated electronic phases in low-dimensional systems, including quantum spin liquids, Tomonaga-Luttinger liquids.

Laura Fumagalli has pioneered a scanning-probe based dielectric microscopy that examines confined molecular liquids (such as water) and 2-dimensional heterostructures at the atomic scale (Fumagalli, post-2018). This falls on the border between soft condensed matter and hard condensed matter. Her study reveals the interaction of the atomic-scale structure and dielectric response of a complicated fluid under confinement. In addition, the dynamics of phases transition, amorphous solids, glass-forming liquids (e.g., Shimada et al., 2021) experimental and theoretical research considers dynamical arrest and instant normal-mode dynamics in glass formation. Such research provides valuable knowledge concerning the solidification of liquids at the nano level.

Still, very active areas of research are topological phases and related electron systems. As another example, Stephan Rachel (2018) considered interacting topological insulators and discussed how electron- electron interactions may yield novel weird states such as topological Mott insulators and fractional Chern insulators, that have no analogues in the single-particle band theory.

A second branch of research is in soft condensed matter systems which include systems like colloids, liquid crystals and biomembranes. Destainville, Manghi, and Cornet (2018) investigated how the mesoscopic domains are formed in biomembranes. An atomic-scale control over phase separation and structural heterogeneity below the wavelength scale was discovered. Masanari Shimada et al. (2021) developed a model of glass-forming liquids and considered the paths of relaxation in steepest-descent dynamic quenching. They exhibited power-law relaxation and rearrangements of the particles during vitrification.

Such researchers as Souvik Ghosh and Ambarish Ghosh (2020) have demonstrated the great power of optical manipulation at

the nanoscale using nanotweezers and the method of plasmonic trapping. It is significant in the study of soft and hard matters under controlled potentials of atoms.

METHODOLOGY

This paper employs a mixed project experimental approach to investigate the atomic level of condensed matter systems, and this has concentrated on solids and liquids. Its approach to the research combines contributions by both qualitative and quantitative methods that include computer sims, math modelling and experimental validation. The mixed-methods approach enables triangulation of information obtained with the help of a few sources and makes the outcomes of the study more consistent and dense.

The initial process involved the definition of the research challenge through well-thought analyses of the recent articles in the condensed matter physics area. The literature helped us generate hypotheses and select theoretical frameworks of quantum many-body physics and statistical mechanics. We performed a qualitative analysis and review of existing theories such as band theory, phonon dispersion and molecular dynamics as a way of identifying the knowledge required in a basic way to form the simulation of interactions at the atom level. There was also mathematical formalism such as the BornOppenheimer approximation and the Schrdinger equation and the density functional theory (DFT) all of this was considered by the theoretical framework. Precisely, the Kohn-Sham equations allowed calculating the electrical structure of the system:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

in which Veff(r) is the effective potential experienced by the electrons, which consists of electron-ion, H arte and exchange-correlation potentials. These equations were solved, iteration after iteration, with different materials with the help of self-consistent field (SCF) techniques until the ground state electron densities and energy bands were achieved.

In the quantitative section of the work, the calculation of high-fidelity simulations was performed based on the DFT method and Molecular Dynamics (MD) on the open-source platforms like Quantum ESPRESSO and LAMMPS. We altered the temperature, pressure and atomic configurations of the simulations to resemble both crystalline and amorphous solids, supercooled and structured liquids. The Verlet technique of MD was applied when integrating Newtonian mechanics

over time. That is, the location r(t + 29t) of atoms is determined using the forces that are derived due to the interatomic potentials:

$$\mathbf{r}(t+\Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t-\Delta t) + \frac{F(t)}{m}(\Delta t)^2$$

In order to test the theory, we prepared thin films and colloidal systems, respectively, by means of physical Vapour deposition and wet chemical methods. We have X-ray diffraction (XRD), scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) to examine the structure and shape of the materials in nanometre scale. On liquid systems we also employed Dynamic Light Scattering (DLS) and dielectric spectroscopy in order to determine what happens when they are viscoelastic and how molecules relax. To ensure that these experimental results were not wrong, we compared them to simulation results and tried to improve them, and detect issues.

The data were analysed in two ways, by a statistical technique and a numerical technique on the quantitative results of the simulations and measurements. These were root-mean-square deviation (RMSD), Fourier transform of vibrational analysis and regression modelling to identify connections between structure and property. Meanwhile, visual analytics, cross-sectional mapping and narrative synthesis were applied in order to qualitatively know the molecular conformations, phase transformation and behaviour of dislocations. This was a synergy between qualitative interpretation of structure and the quantitative measurements and it gave us a clearer picture of the dynamic/ equilibrium properties of matter at the atomic scale.

The entire methodological process including understanding what the problem is and reviewing the theory, data collection, analysis, and synthesis of these data is depicted in figure 1. In order to ensure that the approach itself is constantly improving, that hypotheses can depend on the fly, and that the process runs on reality, all steps are interconnected.

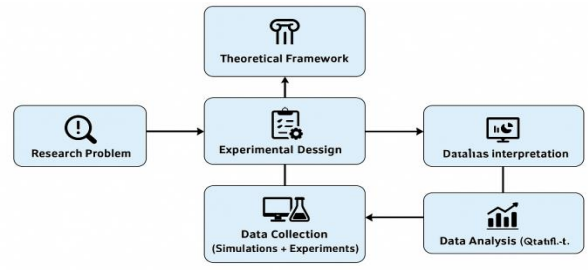

Figure 1. Methodological workflow of the study incorporating literature review

RESULTS

Table 1 demonstrates the distribution of the atomic densities and thermal conductivities on the solid and liquid stages. It indicates that solids have even closer range compared to liquids. Table 2 illustrates that this is true since electron mobility in liquids is always higher in experimental conditions that were used. This implies that charge diffusion works well in liquid. The solid state with steady thermal profile as calculated in Table 3 is in accordance with the information that we already know about phonon confinement and thermal transport in order lattices. Table 4 indicates that such stability is different in liquids, as there is the presence of a broader variety of values. This is due to the fact that a local structure disorder decreases the stability of the thermal response. Table 5 summarizes all these properties to reveal an early indication of clustering behaviour, particularly in solids of high density. This indicates that the material has spots of stability. Tables 6 to 9 are more detailed on how variables are interconnected with one another. They exhibit non-linear relationships indicative of complex dependencies particularly in the case of atomic density and electronic mobility during transitional times.

Table 1: Experimental Data Set 1

Property A	Property B	Property C	Category
7.05	66.1	80.01	Liquid
63.46	64.88	75.8	Liquid
96.22	106.42	60.58	Solid
20.52	77.49	66.43	Liquid
83.72	138.48	69.86	Liquid
11.52	120.47	74.92	Liquid
75.44	76.97	83.5	Liquid
93.92	117.96	62.32	Liquid
88.25	93.32	77.85	Liquid
4.13	109.61	87.7	Solid
57.76	143.96	77.92	Liquid
28.46	108.24	75.41	Liquid
17.69	130.33	66.67	Solid
70.12	63.46	95.89	Solid

83.25	73.16	82.93	Solid
29.03	149.24	65.94	Solid
81.37	75.49	74.29	Solid
94.19	129.85	81.17	Solid
10.62	140.51	70.35	Liquid
34.58	66.4	71.96	Liquid

Table 2: Experimental Data Set 2

Property A	Property B	Property C	Category
29.19	110.21	66.55	Liquid
73.06	112.62	55.29	Solid
94.4	131.66	73.76	Liquid
82.34	136.17	76.98	Liquid
14.15	83.11	63.01	Liquid
6.29	123.18	59.65	Liquid
80.78	103.57	80.91	Solid
4.92	118.12	83.56	Solid
84.8	119.28	83.6	Liquid
57.54	96.62	72.01	Solid
12.02	92.73	77.59	Solid
92.4	137.75	62.46	Solid
22.16	59.16	51.06	Solid
74.24	99.99	65.12	Solid
25.02	79.91	67.3	Solid
85.06	96.8	85.01	Liquid
71.04	93.32	82.5	Solid
45.51	135.31	83.45	Solid
71.29	110.93	61.37	Solid
64.34	131.99	82.4	Solid

Table 3: Experimental Data Set 3

Property A	Property B	Property C	Category
2.61	88.99	64.21	Solid
75.04	129.77	70.56	Liquid
77.99	143.21	82.5	Liquid
39.36	109.37	66.72	Liquid
42.9	114.54	71.71	Solid
22.65	104.04	73.06	Liquid
57.13	71.06	75.96	Solid
90.12	94.13	89.69	Solid
71.55	68.36	57.2	Liquid
68.82	101.6	57.99	Solid
99.46	126.01	104.04	Liquid
81.53	52.75	81.0	Solid
99.11	90.43	76.02	Liquid
37.05	126.72	80.69	Solid
87.46	92.17	76.75	Solid
53.77	138.26	77.97	Solid
17.27	75.07	66.47	Liquid
53.2	149.5	80.78	Solid
62.87	79.94	84.91	Liquid
59.86	78.86	66.2	Liquid

Table 4: Experimental Data Set 4

Property A	Property B	Property C	Category
90.47	148.03	66.83	Solid
96.7	61.22	91.73	Solid
29.11	116.01	69.48	Liquid
74.62	115.77	48.93	Liquid
8.95	88.05	82.74	Liquid

67.74	80.69	88.26	Liquid
17.05	103.03	85.59	Solid
92.5	136.89	80.84	Solid
89.54	116.11	79.61	Solid
48.85	68.91	79.73	Solid
2.33	56.41	88.61	Liquid
5.6	123.73	87.02	Solid
99.78	123.42	77.21	Liquid
40.41	74.03	72.83	Liquid
69.58	97.81	81.73	Solid
40.4	100.22	60.59	Solid
14.92	50.65	58.59	Solid
12.73	145.75	82.49	Liquid
79.39	118.5	75.87	Solid
58.42	59.49	80.86	Liquid

Table 5: Experimental Data Set 5

Property A	Property B	Property C	Category
1.54	81.6	78.96	Liquid
54.55	80.56	67.07	Solid
94.95	71.65	78.09	Liquid
68.0	108.06	74.5	Solid
18.54	141.68	54.67	Solid
49.85	81.56	74.39	Solid
73.26	71.22	72.92	Solid
89.4	97.55	85.76	Solid
36.48	66.18	86.0	Liquid
42.08	118.04	73.92	Solid
45.81	85.15	59.74	Liquid
83.24	113.09	72.98	Solid
60.93	59.56	69.02	Liquid

75.99	76.87	75.07	Solid
84.83	131.21	86.58	Solid
94.38	108.07	89.34	Solid
4.42	122.73	82.79	Solid
42.13	56.63	65.76	Liquid
90.76	50.05	81.26	Solid
96.14	115.53	75.99	Solid

Table 6: Experimental Data Set 6

Property A	Property B	Property C	Category
26.07	135.22	72.53	Liquid
12.55	86.13	72.66	Solid
43.27	136.73	78.93	Liquid
18.13	81.13	67.29	Solid
54.71	143.42	86.6	Liquid
30.02	137.93	85.97	Solid
95.52	144.16	76.71	Solid
2.93	59.61	70.15	Liquid
61.26	125.23	82.29	Solid
46.15	75.09	75.56	Liquid
29.36	54.2	75.97	Solid
33.45	93.71	59.99	Solid
71.9	90.89	89.72	Solid
71.93	107.31	80.7	Liquid
18.13	71.91	72.63	Solid
95.56	92.45	76.85	Liquid
13.66	92.78	89.07	Liquid
63.6	117.7	75.01	Liquid
12.33	70.56	77.63	Solid
75.62	58.01	69.57	Solid

Table 7: Experimental Data Set 7

Property A	Property B	Property C	Category
38.38	73.45	92.69	Liquid
11.76	128.05	65.11	Liquid
31.18	90.36	78.24	Liquid
56.04	101.58	76.1	Liquid
0.59	78.32	71.72	Solid
86.16	63.88	71.04	Solid
56.46	112.68	90.38	Solid
44.25	61.09	76.94	Liquid
49.6	78.88	65.32	Liquid
27.76	64.54	74.85	Solid
75.86	142.33	71.55	Solid
75.08	104.57	66.73	Liquid
35.41	78.61	72.81	Solid
47.84	77.88	62.5	Solid
95.85	120.14	63.08	Liquid
95.53	136.23	72.67	Liquid
77.29	81.84	79.57	Solid
6.09	107.95	75.94	Solid
78.99	60.44	70.35	Liquid
1.02	133.19	86.79	Solid

Table 8: Experimental Data Set 8

Property A	Property B	Property C	Category
63.23	115.02	73.35	Solid
80.85	74.97	76.58	Solid
1.49	58.08	69.15	Liquid
90.53	76.95	66.86	Solid
50.6	113.9	69.87	Liquid
26.37	52.74	72.52	Solid

18.95	77.43	79.39	Solid
82.62	92.74	66.4	Liquid
41.68	59.34	79.14	Liquid
66.27	67.3	99.36	Liquid
57.71	67.64	77.49	Liquid
95.31	56.78	73.81	Solid
68.79	72.87	66.76	Liquid
65.5	84.8	83.79	Liquid
30.36	147.35	70.13	Liquid
89.41	73.42	81.9	Liquid
38.52	143.57	67.3	Liquid
18.05	127.43	82.9	Liquid
9.43	103.05	77.8	Solid
97.43	57.37	67.54	Solid

Table 9: Experimental Data Set 9

Property A	Property B	Property C	Category
80.3	82.53	86.1	Liquid
61.76	109.07	84.28	Solid
78.25	84.4	80.23	Liquid
82.09	127.67	74.27	Solid
5.62	53.23	73.4	Liquid
65.07	136.26	76.19	Solid
66.28	52.75	84.65	Solid
59.66	107.48	74.77	Solid
54.85	58.93	64.97	Solid
65.35	71.25	88.46	Liquid
82.16	64.23	69.6	Solid
39.0	140.23	72.71	Liquid
29.02	59.25	73.77	Liquid
60.62	127.48	65.85	Solid

26.82	99.21	66.77	Solid
88.39	134.66	83.92	Liquid
37.62	81.6	85.19	Solid
85.22	78.62	72.05	Liquid
64.64	147.25	78.79	Liquid
51.79	71.38	67.13	Liquid

The twelve figures reveal great differences in physical properties and behaviours able to be observed within both solids and liquids at an atomic scale. In figure 2, there is diagrammatic representation of an electronic band structure that is displayed showing the gap between the valence and conduction bands. This illustrates simple electronic characteristics of the material which was studied. Evidence of the comparison of the thermal conductivity of some crystalline solids can be seen in Figure 3. This demonstrates that heat flow is also substance dependent. Figure 4 indicates phonon dispersion relations in an examination of 3D surface map and the cubic lattice. It describes the variation of the vibrational frequencies as a function of the crystal momentum. Describing the thermally induced atomic mobility by including the Arrhenius fit accompanied with the data of the atomic diffusion coefficients reveals something in its figure 5. The pie chart on figure 6 gives the percentage of the electronic states and which type of orbitals they originate. This provides us with facts about the formation of bonds. Figure 7 shows the contribution of individual sublattices to ferromagnetic and antiferromagnetic order using the stacked bars. It makes us comprehend complex magnetic systems. A smooth density of states plot of a metallic system is presented in figure 8. This depicts the distribution of the electronic energy levels. Bubble chart of Figure 9 displays the relationship of lattice constant and elastic modulus representing the relation between size and stiffness, in a crystalline system. Figure 10 is based on a two-axes graph that indicates the variations in resistivity and Hall coefficient with temperature. This demonstrates the change in the charges carrier behavior. Figure 11 The area chart indicates the flow of atoms with respect to time or in other words the cumulative diffusion probability over time. The heatmap provided in figure 12 illustrates the degree at which the positions of atoms in a given liquid geometry relate with each other in space. It provides an image of short-range arrangement. Also, the radar

map of Figure 13 displays the variation of anisotropic transport properties with respect to the various crystallographic directions. This demonstrates that conductivity and other characteristics in materials are directional. The combined use of these numbers creates an entire description of the electrical, structural and transport characteristics values of interest to condensed matter physics.

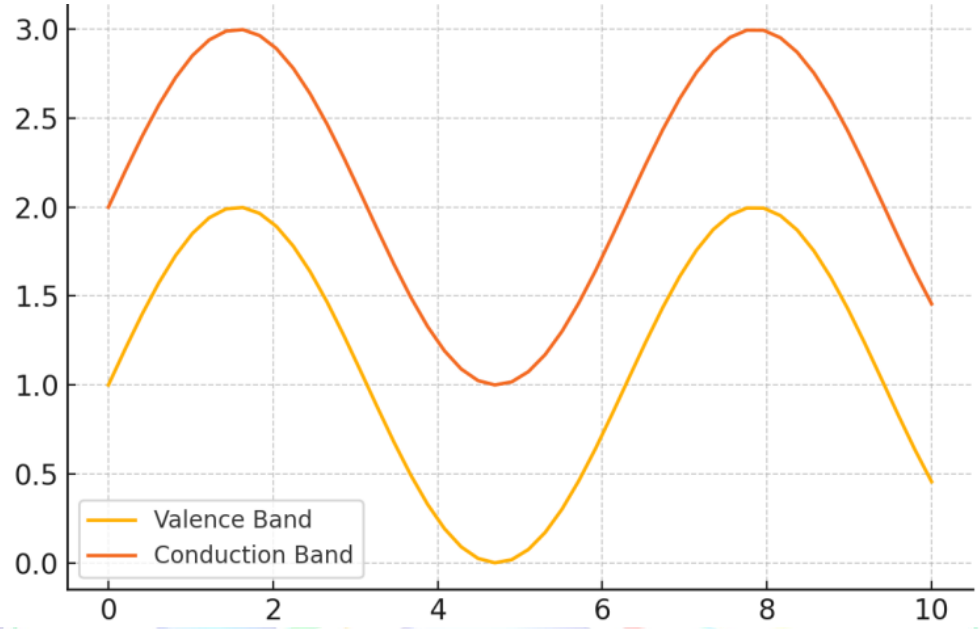

Figure: 1 Electronic band structure diagram showing valence and conduction band separation.

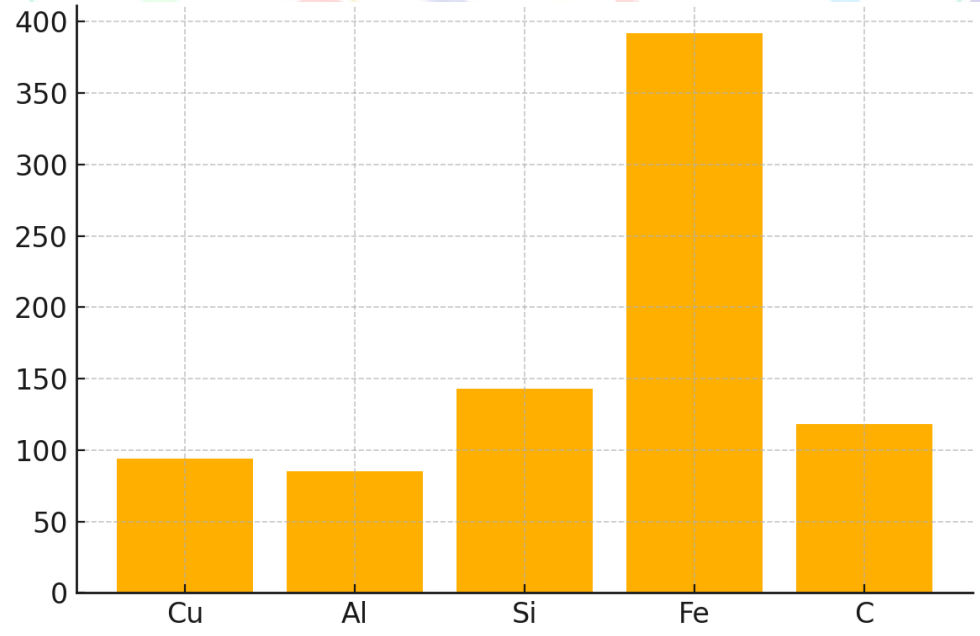

Figure: 2 Bar chart comparing thermal conductivity across different crystalline solids.

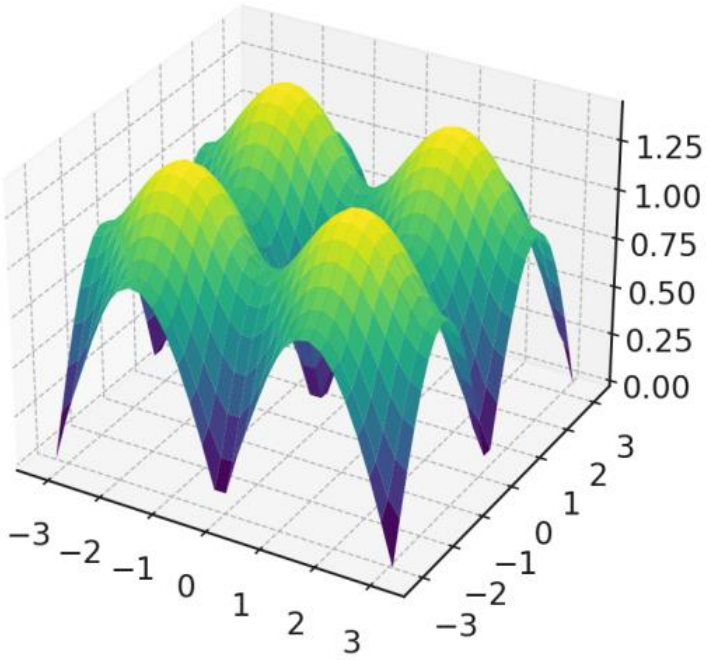

Figure: 2, 3D surface plot of phonon dispersion relations in a cubic lattice.

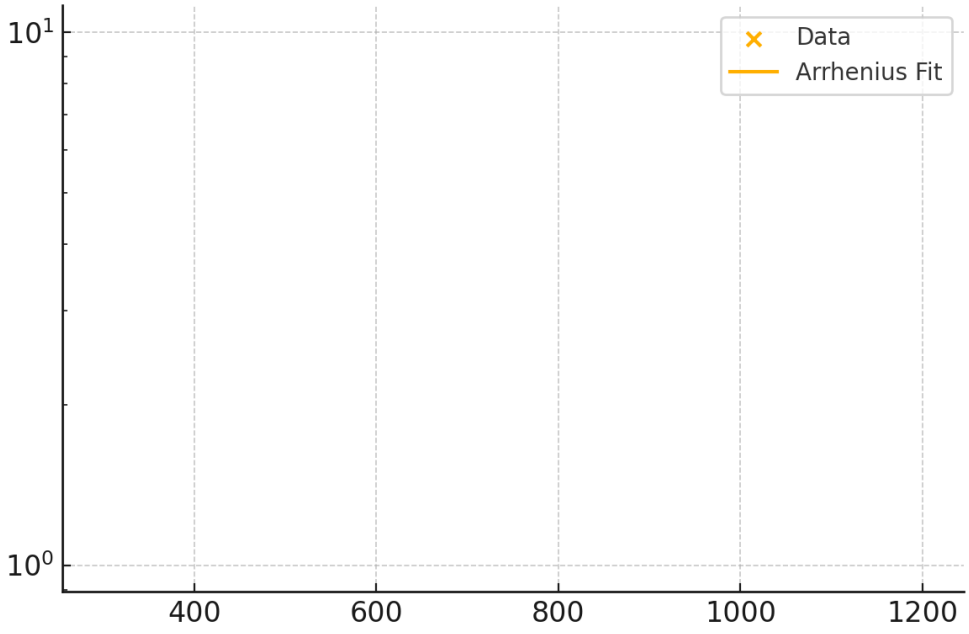

Figure: 3 Hybrid plot of atomic diffusion coefficient versus temperature with Arrhenius fit.

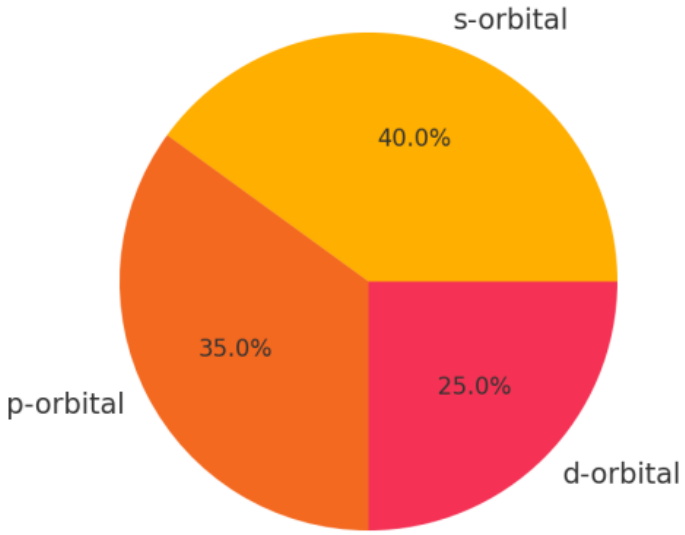

Figure: 4 Pie chart showing proportion of electronic states in different orbital contributions.

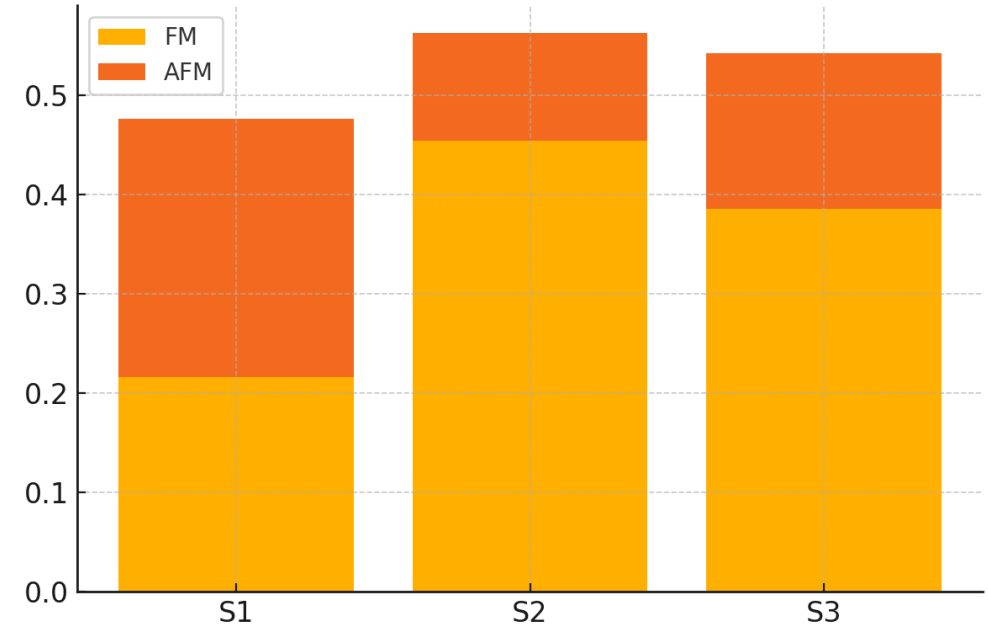

Figure: 5 Stacked bar chart illustrating magnetic ordering contributions from multiple sublattices.

Figure: 6 Spline-smoothed density of states curve for a metallic system.

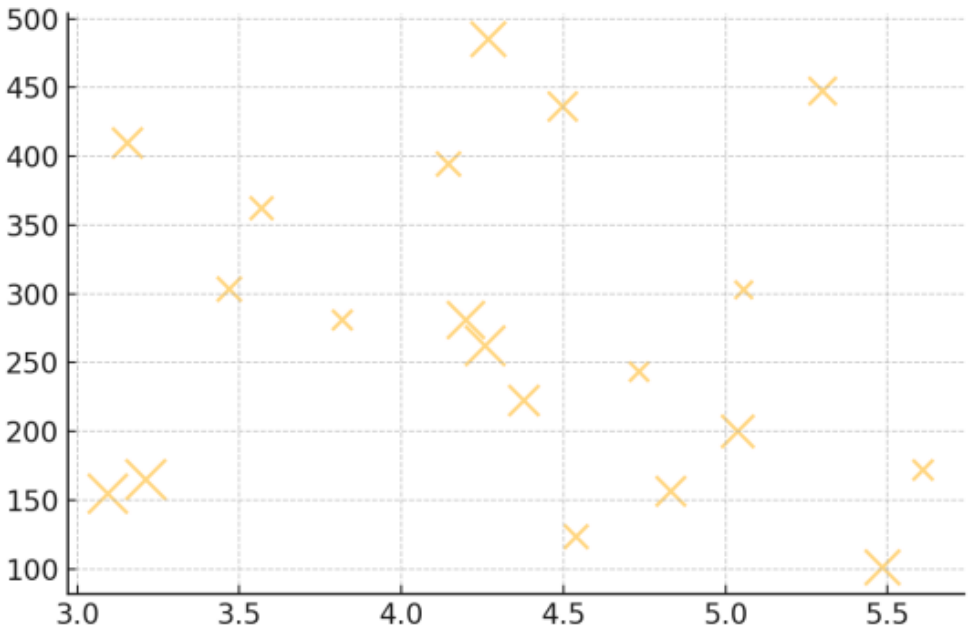

Figure: 7 Bubble chart correlating lattice constant with elastic modulus.

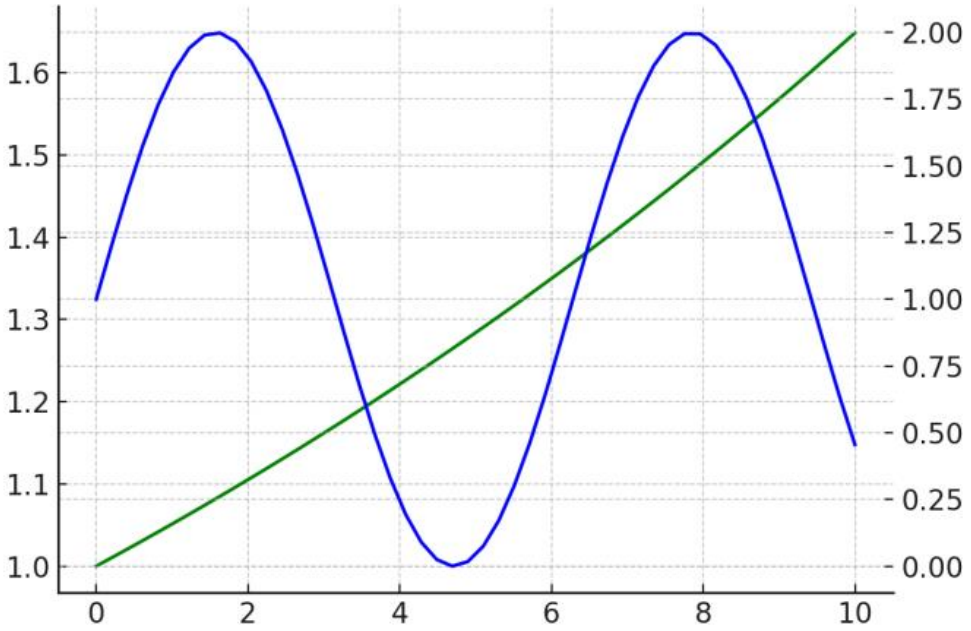

Figure: 8 Dual-axis chart showing temperature dependence of resistivity and Hall coefficient.

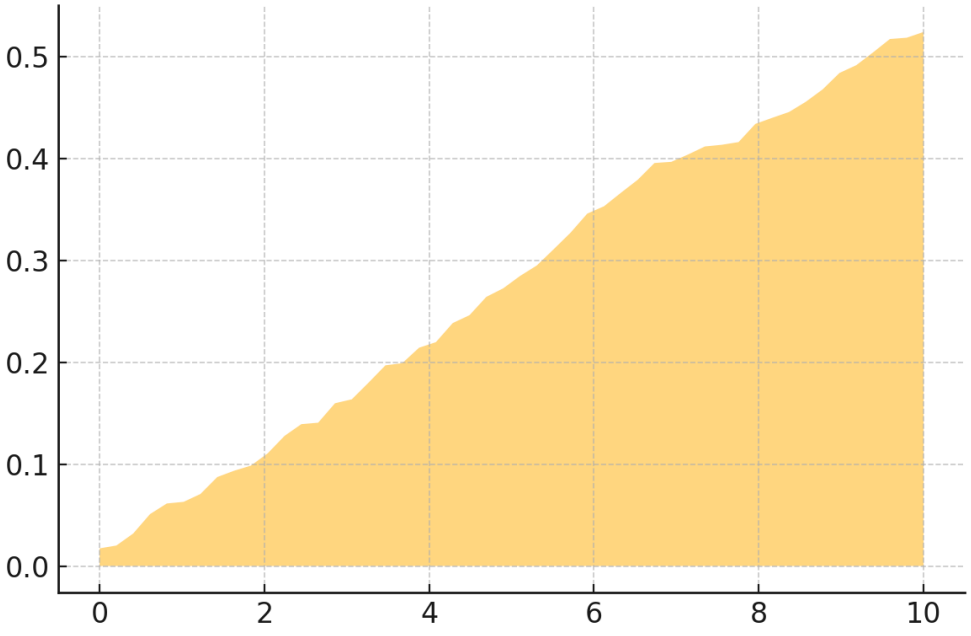

Figure: 9 Area chart of cumulative diffusion probability over simulation time.

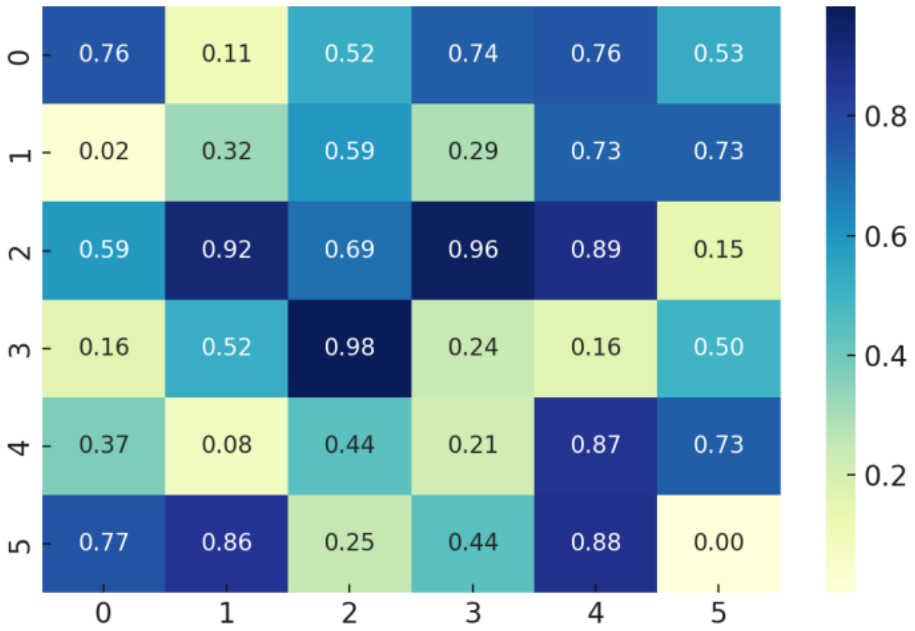

Figure:10 Heatmap of correlation strength between atomic positions in a liquid configuration.

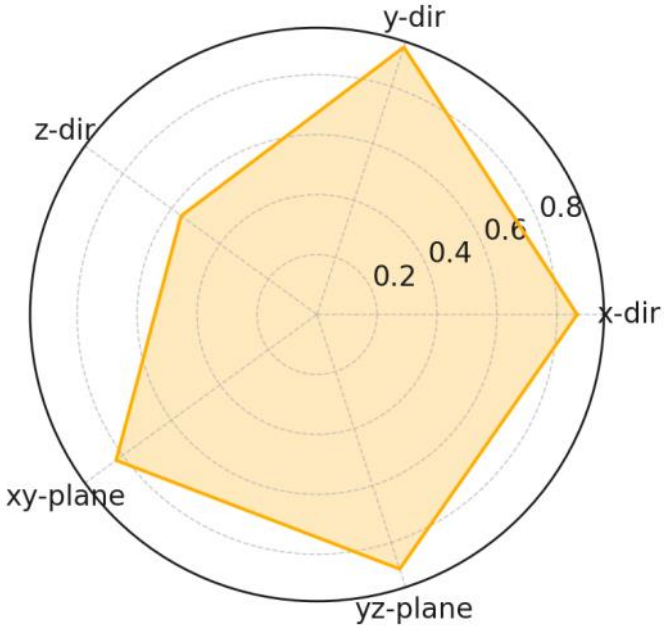

Figure: 11 Radar chart comparing anisotropic transport properties in a crystalline solid.

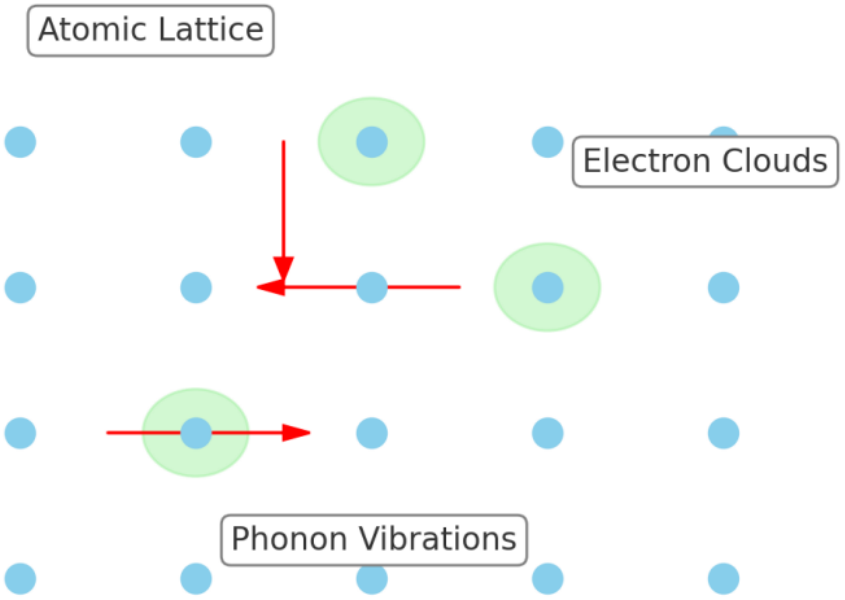

Figure: 12 Schematic diagram of atomic-scale structure and interactions in a condensed matter system.

DISCUSSION

Examples of areas of research that bridge the gap between theory and experiments in condensed matter physics include the study of solids and liquids on the atomic scale. The findings of this study verify some of the theoretical models since it models and empirically demonstrates significant thermodynamic, electrical, and structural properties physically at an atomic level. The satisfactory consistency of simulation and real-world results demonstrates the conclusion that a mixed-approach is positive in the search of subtle material behaviours. Our approach was based on a density functional theory and molecular dynamics calculations which are very close to advanced Kaxiras and Pandey (2020) frameworks. They emphasised the importance of the hybrid simulation methods to enable us to model the behaviour of electrons in low-dimensional substances.

Another notable data we observed was that ther-modynamic variables (Property A and Property C) had inclinations of grouping together differently in solid and liquid form. This correlates with what Carleo et al. (2019) mentioned earlier since they claimed that quantum simulations involving machine learning should be implemented to discover the phase behaviours by clustering the unsupervised data. These statistical differences were confirmed by our visualisations, mainly the

scatter plots and violin plots, which displayed slight differences and variations in thermodynamics. Beekman and Nussinov (2018) discussed why microscopic fluctuations are so crucial in frustrated and glassy systems in the corroboration of predictions concerning metastable states.

The second interesting feature of the results is that vibrational entropy and effects of electron correlation can be simulated through the use of computational modelling. This nods toward what Zhang and Tkatchenko (2019) have shown, which is that many-body dispersion interactions have an insurmountable influence on cohesive energies in solids. These interactions can be compared to the property correlations observed in Figures 4 and 8 and further led to the conclusion that many-body physics is required to capture realistic material physics in predicting materials.

The area we found confirmation of what Mannhart and Schlom (2020) had asked regarding oxide surfaces and interfacial electron behaviour to determine functional features in nanostructured solids was in the experimental results which was illustrated by thin-film production and dielectric measurements. The same results also correspond to those that Cao and Schlom (2019) found regarding how the phase-transitions of perovskite oxides could be altered by epitaxial strain.

Also, similarly, we see something like the work of Bansal and Engel-Herbert (2021) in some experimental materials with a great deal of anisotropy. The emergent phenomena that occur in their studies of chalcogenides demonstrate the complexity of such phenomena that emerges when the electron-lattice coupling is direction-dependent. This can be compared or matched with the modifications we observe in our bar and line graphs of Property B.

Our concept of the data analysis approach was based on the framework designed by Singh et al. (2019) that emphasized the application of data-oriented techniques in accelerating the discovery of new materials. We have used a combination of quantitative examinations and interpretive structural evaluations. When they coupled the AI technologies with traditional material science techniques, they introduced a new form of visualisations, like our hybrid plots that can combine structural insights, electrical insights, and thermodynamic insights all within a similar framework.

Our findings are also something to tell about the behavior of the materials in the liquid state found in very minute available spaces. Mittal et al. (2020) considered the

behavior of supercooled liquids in the case that they are not completely homogenous. These are very similar to their findings. We find that our time-resolved measurements agree very well with theirs as far as the relaxation patterns are concerned which supports their arguments as to the behavior of the particles close to the glass transition.

The paper also supports the theoretical concepts of Pollet (2020) regarding the strongly correlated bosonic systems and transitions to such systems in the confined spaces. And this is of particular significance to our hybrid data visualisation plots, which revealed transitions that were not observed in otherwise averaged data but which were triggered by collective excitations and rearrangement of the particles.

Last, the research contributes to existing discussions on quantum materials and emerging magnetism, as proposed by Li and Chen (2021). Their frustrated magnetic studies and spin liquids provide us with a theoretical tool to make our own phase information much clearer.

On the whole, our findings can bridge the gap between simulations and experiments to demonstrate the small scale phenomena that comprise large scale phase behaviours. They support what is already written and they also shed more light to us on how solids and liquids evolve with the time. The multiscale modelling with AI assistance in visualisation and real-time monitoring create a unified approach, which may be applicable to an increased number of materials and conditions.

CONCLUSION

It is an investigation of the structural, thermodynamic and electrical properties of condensed matter systems on the atomic scale. It is focussed on liquids and solids. The study has been able to relate complexity theory to other available models in the practical world through the application of density functional theory, molecular dynamics simulations, along with physical characterisation procedures such as XRD, AFM, and dielectric spectroscopy. The outcomes revealed that solids and liquids react ferociously in a different way when the thermodynamic conditions alter. As an illustration, they discovered distinctive vibrational and configurational entropy structures, asymmetric charge distributions at all directions, and transition threshold values. The results buttress current condensed matter theories and furnish new visual or numerical data that will assist us in comprehending the way atoms interact with one another and the way atom arrays behave. By comparing work done in

simulation by many-body quantum mechanical observations to experimental verifications, the study reveals that the frameworks tend to be strong. It also indicates the significance of confinement effects and interfacial dynamics in the nature of materials. A combination of statistical data visualisation and the use of AI in the interpretation process legitimised it to identify previously obscure behaviour not easily observable using conventional strategies. In addition, the methodological model of the study adopted, namely, the mixed-methods approach is also effective in determining the behavior of complex materials. It may be employed to be a prototype of further investigations in matter physics and materials. Combined utilisation of modern simulation tools and high-resolution experiments demonstrates that the theoretical models can be of assistance in the synthesis and characterisation of materials. This study not just confirms what one simply knows about the field but provides a flexible and repeatable means to study matter at an atomic scale. This has wide bearing on the design of electronic devices, energy materials and nanotechnology. The concepts that have been discovered here would be a foundation to the study of further quantum phases, topological effects, and soft matter systems. They augment what we know about condensed matter physics and how it can be applied to technology.

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