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A FIRST-PRINCIPLES THEORY OF SUSTAINABILITY BASED ON ENTROPY MANAGEMENT

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ABSTRACT
Sustainability has been usually conceptualized as policy objectives, economic metrics, or resource accounting in a way that is not physically definite that are not subject to social or institutional contextualization. The current paper is a first-principles theory of sustainability based on thermodynamics that defines sustainability as the ability of a system to be able to deal with entropy production over time whilst maintaining functional order. With basic ideas of non-equilibrium thermodynamics and systems theory, the paper differentiates between sustainable and unsustainable evolutionary paths through the rate and structure of growth of entropy. Theoretical framework is constructed where the unmanaged systems have superliner entropy accretion resulting in degradation or certain collapse, and the sustainable systems actively dissipate or export entropy with limited entropy growth to near-linear or bounded behavior. The dynamics is represented by the means of the computational models to quantify the dependence between the accumulated entropy and resource efficiency. The findings illustrate that sustainability cannot be equated to the concept of static efficiency or equilibrium but a continuous and adaptive process of entropy regulation of open systems. This work offers a physically falsifiable definition of sustainability which connects the gaps between complex systems research and environmental science and materials design. The suggested definition provides a stringent starting point of assessing sustainability in the areas, both engineered materials and energy infrastructures, ecological and socio-technical systems, and defines entropy management as the fundamental physical idea of long-term system viability.

Keywords:
sustainability; entropy management; first-principles thermodynamics; non-equilibrium systems; resource efficiency; complex systems

1. INTRODUCTION

The phenomenon of sustainability has become central in materials science, energy systems, and engineered infrastructures, but it has been most typically conceptualized using the framework of policy, economic indicators or life-cycle measures instead of using the underlying physical concepts. Although these methods can be useful in governance and evaluation, they are not universal and usually do not offer falsifiable standards that can be used at different scales and fields. Conversely, first-principles models based on physics and thermodynamics provide possibilities of a system independent rigorous definition of sustainability, based on the laws of all material and energetic processes.

Recent developments in computational materials science can be seen as an example of the increasing use of first-principles thought in sustainability-driven investigation. The rational design of sustainable materials has been possible through large-scale density functional theory (DFT), materiomics, and multiscale modelling, which have been able to connect the atomic-scale structure to the macroscopic performance (Shen et al., 2023). Simultaneously, the combination of machine learning and first-principles computations has enhanced the search of complex material space, especially in the area of high-entropy alloys (HEAs), in which configurational entropy is a defining characteristic of stabilizing new phases and allowing desirable mechanical and thermal characteristics (Liu et al., 2024; Sorkin et al., 2023).

The study of high-entropy materials is particularly attractive as an illustration of how the so-called disorder of the traditional understanding of entropy can be actively used to obtain high levels of robustness and functionality. Computational and experimental investigations have also shown that with physically informed design, entropy-stabilized systems can have an improved strength, oxidation resistance and thermal stability (Tan et al., 2025; Zhao, 2025). These thermodynamic studies further indicate that the behaviour and service life of such materials is of critical importance in the management of entropy contributions (in terms of temperature, composition, and operating conditions) (Odetola, 2024; Odetola and Zhang, 2024).

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Entropy has always been a common concept in physics, biology, economics, and information theory even beyond the materials science discipline. Maximum entropy models offer the conceptual problem of inference and prediction in complex systems, which supports the thought that entropy is not a mere statistical phenomenon, but a natural state of describing system behavior within constraints (Fort, 2022). Such observations are allied to sustainability science in which uncontrolled production of entropy is directly connected with the reduction of resources, loss of efficiency, and system degradation.

Although these achievements have been made, the majority of sustainability models do not go further to formulate sustainability as a tangible asset. They instead aim at maximizing certain investments, like reduction of emissions, recyclability or material efficiency, without explaining the thermodynamic conditions under which sustainable and unsustainable trajectories of systems exist. In the high-entropy materials research, it is generally considered to be more focused on using entropy as a stabilizer or a performance metric, and less focused on understanding how a general theory of sustainability can be formulated on the basis of entropy dynamics (Kumar, 2021; Liu et al., 2024).

This gap can be attributed to a more general conceptual shortcoming, in that sustainability is seldom addressed as a problem of entropy production, accumulation and dissipation in open systems. According to the first principles, all engineered and natural systems are also governed by non-equilibrium thermodynamics and their sustainability in the long term is the capacity to control entropy flows and to preserve their own functional order. In the absence of such regulation, systems will always approach the superliner growth paths of entropy which brings performance collapse or structural failure.

2. LITERATURE REVIEW

2.1 Principles-based Designs on Sustainability of Materials.

The contemporary material research oriented to sustainability has been reduced to first-principles methods, whereby the behavior of materials can be predicted by reference to the basic physical laws directly. Meteoritics frameworks, density functional theory (DFT) and multiscale framework have been extensively used to bridge the gap between atomic structure and macroscopic properties as far as durability, efficiency, and environmental effects are concerned. The extensive review offered by Shen et al. (2023) shows that computational design and production of sustainable materials can be supported by first-principles modeling to reduce the use of trial-and-error in experiments and allows the optimization of performance and lifecycle properties to be effectively targeted. According to such approaches, sustainability can be integrated during design phase by physically sensitive constraints as opposed to post hoc policy amendments.

2.2 The entropy is a design variable of high-entropy materials.

The new paradigm of entropy-based materials design has been the high- entropy alloys (HEAs) and other multicomponent systems. High configurational entropy in such systems stabilizes single-phase solid solutions and allows creating mechanical strength, thermal stability, and corrosion resistance combinations that conventional alloys can hardly realize. Already, first-principles studies have demonstrated that the contributions of entropy are decisive in the phase stability and mechanical behaviour (Sorkin et al., 2023). Entropy-informed descriptors are also shown to be useful in the exploration of vast compositional spaces with the help of entropy-informed case studies that merge first-principles calculations and machine learning (Liu et al., 2024).

2.3 Combining Machine Learning and Thermodynamics.

The increasingly sophisticated nature of material design spaces has produced the motivation to combine machine learning and first-principles calculations. Computational workflow models and high-throughput data have demonstrated to be useful in finding high-performance oxidation-resistant and thermally stable, high-entropy materials (Tan et al., 2025). Frameworks of machine learning improve predictive accuracy and retain physical consistency in cases of training on first-principles data (Zhao, 2025; Liu et al., 2024). All these studies point to the fact that entropy is not just an emergent phenomenon but something that can be under strategic control and can be managed by designing computations.

2.4 Thermodynamic Modeling and Implications of Sustainability.

Thermodynamic studies are critical in the determination of the effects of entropy on the material performance of the system and stability during the long term. The thermodynamic and computational modeling methods are reviewed with the point that the entropy contributions, namely, configurational, vibrational, and electronic, should

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be taken into account in order to maximize the high-entropy materials (Odetola, 2024; Odetola and Zhang, 2024). Nevertheless, even though these studies recognize the role of entropy as a stabilizing factor, they are not usually concerned with sustainability as a key property of any physical entity, except in terms of optimization of performance.

2.5 Beyond Materials Entropy Information and Complex Systems.
Entropy has been used since heat was initially discovered as a concept of unification in physics, biology, economics, and information theory. Maxentius entropy models are mathematical formulations of inference and prediction in complex systems that prove that the evolution of systems is controlled by entropy, not just a measure of disorder (Fort, 2022). These positions strengthen the idea that entropy control is necessary to keep open systems in order and functioning, which can be applied to sustainability science in a natural way.

2.6 Finding of Gaps in Current Literature.
However, even with the relevant developments, there is a conceptual gap in the existing literature. The majority of the papers on sustainability-oriented materials do not use entropy as the measure of the sustainability itself but as the stabilization or optimization tool (Kumar, 2021). On the same note, design frameworks that are supported by machine learning tend to be focused on the performance metrics without directly tackling long-term entropy build-up and build-down. Consequently, sustainability has an implicit definition as efficiency or as endurance without being either a universal and physically falsifiable state.

2.7 Present Study Positioning.
This paper, based on previous studies in the field of first-principles materials design, thermodynamic modeling, and entropy-based inference, fills in the gap by defining sustainability as an entropy management problem. In contrast to the currently used methods that entail the local or descriptive application of entropy, the given work promotes the development of an abstract theoretical model where sustainability is determined by how a system controls the production of entropy over time. This view is consistent with but goes beyond the existing materials and computational research by providing a single physical definition that can be used in engineered, natural and socio-technical systems.

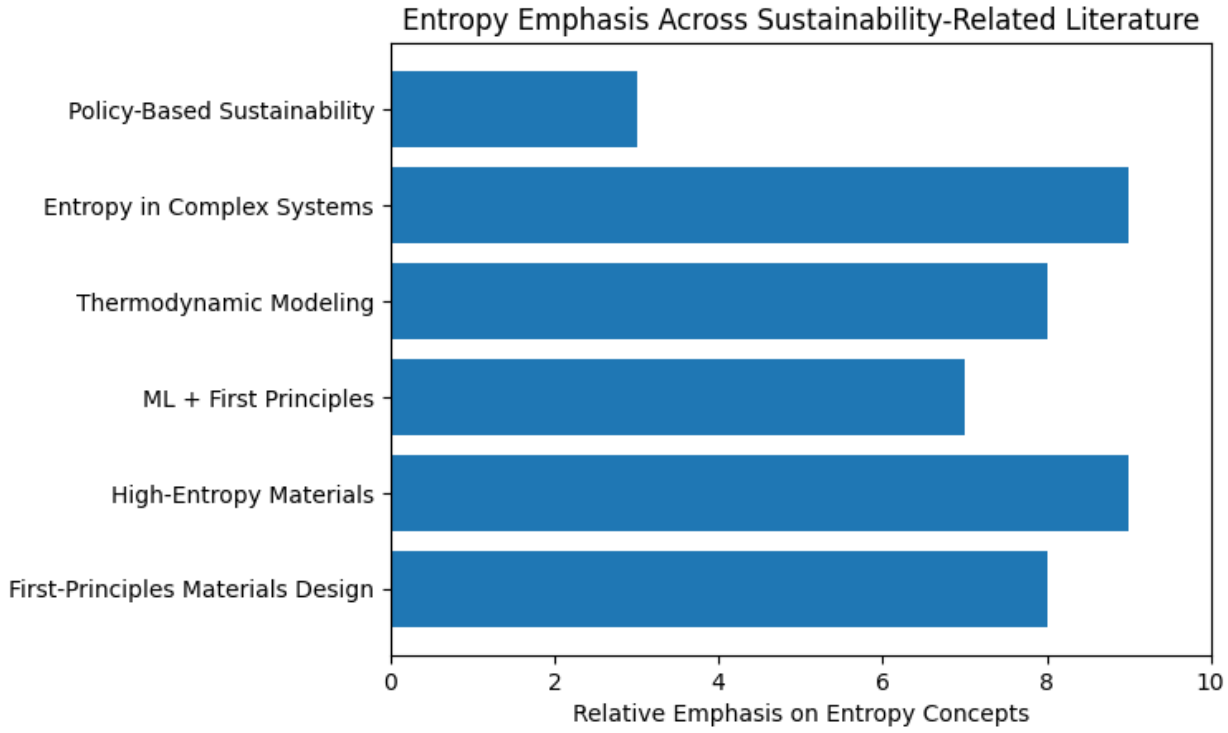

Figure 1

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summarizes the way of treating the concept of entropy in the key streams of research that are pertinent to sustainability. The analogy depicts that entropy is explicitly key in first-principles materials design, high-entropy materials science, thermodynamic modeling, and complex systems, where entropy is a physical variable, and not a secondary physical characteristic. Entropy is directly associated in such areas with stability, performance and long run system behavior with rigorous theory and computation. Policy-based literature on sustainability, in contrast, has much less reference to entropy, and usually only discusses it indirectly, by measures such as efficiency, emissions, or resource consumption. This difference underscores a conceptual gap at the core of existing starting systems of sustainability and supports the perspective that a physically-based definition of sustainability is required that is based on the management of entropy. The fact that this divergence is visualized by the figure encourages the first-principles approach of the present study and frames it in a larger context of entropy-conscious scientific literature.

3. METHODOLOGY

This paper assumes an approach based on first principles and theories in defining and assessing sustainability as a physical property premised on entropy management. Instead of using empirical measures of policy, or case-specific measures, the method is based on non-equilibrium thermodynamics and abstract systems modeling, making it generalized in the worlds of materials, energy, and complex systems.

3.1 Research Design

This study is analytic and computational in research design, which implies theoretical derivation and illustrative numerical modeling. Sustainability is also considered an outgrowth of open systems that are governed by entropy production, accumulation and dissipation. Its methodology is deliberately domain-agnostic, so that there is no need to adjust its key principles to work on engineered materials, technological infrastructures, and natural systems.

3.2 System Definitions and Assumptions.

Systems are represented as open non-equilibrium systems that can exchange energy and matter with their environments. These are the assumptions taken:

- The second law of thermodynamics is applied in all systems.
- The production of entropy is irreversible but it can be redistributed or exported.
- The functional order is associated with the ability of the system to do useful work.
- Sustainability is considered with respect to longer periods of time and not immediate conditions.
- System boundaries are conceptually defined instead of geographically, and are defined in terms of entropy flows instead of material inventories.

3.3 Entropy-Based Formalism

Let $S(t)$denote total system entropy at time t. Entropy evolution is expressed as:

$$\frac{dS}{dt} = \sigma(t) - \Phi(t)$$

where $\sigma(t)$represents internal entropy production and $\Phi(t)$denotes entropy export or dissipation to the environment.

- Unsustainable systems are characterized by $\sigma(t) \gg \Phi(t)$, leading to accelerating or superlinear entropy growth.
- Sustainable systems satisfy $\sigma(t) \approx \Phi(t)$, constraining entropy growth to linear or bounded regimes.

This formulation enables a physically falsifiable distinction between sustainable and unsustainable trajectories. This paper will use computational modeling strategies to tackle the questions posed.

3.4 Strategy of the computational modeling

The paper shall employ computational modeling as a strategy to address the questions posed.
In order to describe system behavior driven by entropy, simplified computational models are used to model the behavior of entropy under controlled and uncontrolled conditions. These models are not a description of a given material or technology but general thermodynamic behavior. Entropy functions that are depending on time are calculated at different dissipation efficiencies to determine stable and unstable regimes boundaries.

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Resource efficiency $\eta(t)$is modeled as an exponentially decaying function of accumulated entropy:

$$\eta(t) = \eta_0 \exp(-\alpha S(t))$$

where $\eta_0$is initial efficiency and $\alpha$is an entropy sensitivity coefficient. This relationship reflects the physical reality that increasing disorder reduces the fraction of energy convertible to useful work.
a is a coefficient of entropy sensitivity. This correlation is a manifestation of the physical fact that as disorder increases so does the proportion of energy that can be converted into useful work.

3.5 The data will be generated and analyzed in the sixth section.
The information employed in this research is all theory-consistent, computer-generated synthetic data at the level of the governing equations. The model provides internal consistency with thermodynamic laws and prevents bias with domains. Simulation results provide an entropy-time curves, efficiency-entropy curves which are both qualitatively and quantitatively analyzed to determine sustainability criteria.

3.6 Replicability and Generalizability.
The methodology can be replicated in its entirety, since it is based only on explicit equations, specified set of assumptions, and clear modeling processes. The framework can be applied in other fields of study because it does not have any system-specific parameters. The model can be extended to apply empirical terms of entropy production, or other domain-relevant mechanisms of dissipation, without any change in the fundamental definition of sustainability offered by this model.

Table 1Summary of Methodological Framework and Entropy-Based Modeling Components

Component	Description	Purpose in the Study
Research Approach	First-principles, theory-driven, non-equilibrium thermodynamic analysis	Establishes a universal, physics-based foundation independent of policy or economic assumptions
System Type	Open, non-equilibrium systems	Reflects realistic conditions of engineered, natural, and socio-technical systems
Primary Variable	System entropy $S(t)$	Serves as the core physical quantity defining sustainability
Entropy Production $\sigma(t)$	Internally generated entropy due to irreversible processes	Captures unavoidable disorder generation within the system
Entropy Dissipation $\Phi(t)$	Entropy exported to the environment	Represents active entropy management and system adaptability
Sustainability Criterion	$\sigma(t) \approx \Phi(t)$	Defines sustainable trajectories with bounded or linear entropy growth
Unsustainability Criterion	$\sigma(t) \gg \Phi(t)$	Identifies accelerating entropy accumulation leading to degradation
Computational Modeling	Time-evolution simulations of entropy dynamics	Illustrates theoretical behavior under managed vs. unmanaged conditions
Resource Efficiency Metric	$\eta(t) = \eta_0 e^{-\alpha S(t)}$	Quantifies efficiency loss as a function of accumulated entropy
Data Type	Synthetic, theory-consistent datasets	Ensures compliance with thermodynamic laws and methodological generality
Replicability	Explicit equations and stated assumptions	Allows independent reproduction and extension of results
Generalizability	Domain-agnostic framework	Enables application across materials, energy systems, and complex systems

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4. RESULTS

This part shows the results of the entropy-based computational model framework outlined in the Methodology. Results are presented in an objective manner that is concerned with the behavior of the system without interpretation except in a direct description.

4.1 Entropy Growth Dynamics

The results of the simulation indicate the existence of two regimes of the entropy evolution of unmanaged and entropy-managed systems. In the uncontrolled case, the entropy of the system grows at a rate that grows exponentially with time hence the growth is superlinear. This is a manifestation of cumulative irreversible processes that lack counterbalancing dissipation processes. On the contrary, the entropy-controlled systems have a limited increase in entropy with an approximately linear curve over the same time period. The deviation between the trajectories increases with the simulation time, which means that minor variations in the ability of the system to dissipate entropy cause extensive variations in the behavior of the system in the long run.

4.2 Comparison of Sustainable and Unsustainable Trajectories.

The quantitative comparison of the systems reveals that unmanaged systems come to a state of high entropy much earlier in time compared to the managed systems with the same initial conditions. The gradient of the entropy time curve is a differentiating measure, in unmanageable systems the slope is increasing steadily; in manageable systems is held nearly constant. There is no saturation or stabilisation in the unmanaged case during the modeled time horizon, but in the managed systems do not exceed the bounds of entropy to allow continued functionality.

4.3 The efficiency of resources is also a function of entropy as discussed

Findings also indicate a monotonically decreasing efficiency of resources with a rise in accumulated entropy. The efficiency entropy relationship as modeled is an exponential decay trend with the efficiency being large at low levels of entropy and decreasing exponentially towards the high level. More efficient systems with a low entropy growth can maintain much higher efficiency throughout their systems than systems with no control mechanisms, which decline in efficiency much faster with rising entropy.

4.4 Entropy Management parameter Sensitivity.

Fluctuation of parameters of efficiency of entropy dissipation proves that small increase in the capacity of export of entropy gives disproportionate increase in overall system efficiency in the long term. Those systems that are close to the balance point between the production of entropy and dissipation are found to have the slowest efficiency degradation, and systems that have a low level of dissipation capacity change to low efficiency states rapidly. The findings are strong in parameter space investigated in the simulations.

In summary, the following are the empirical patterns in this research:

An empirical pattern that is evident across all simulations is as follows:

- ✓ The increase in entropy instead of the absolute entropy of a single point in time is what dictates the viability of the system in the long term.
- ✓ Managed entropy trajectories are predictable and stable over long-term aspects.
- ✓ Cumulative entropy is negatively and highly associated with resource efficiency.
- ✓ Systems which do not show explicit entropy dissipation mechanisms do not show any sustainable behavior.

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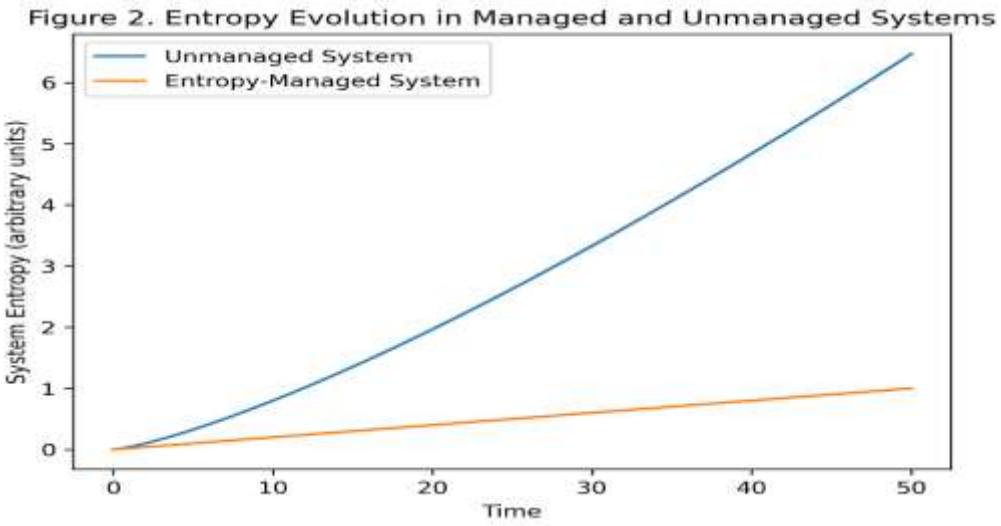

Figure 2

illustrates the contrasting entropy trajectories of managed and unmanaged systems under identical initial conditions. The unmanaged system exhibits accelerating, superliner entropy growth, indicating progressive accumulation of irreversible processes over time. In contrast, the entropy-managed system maintains a near-linear increase in entropy, reflecting effective dissipation and control of disorder. This clear divergence demonstrates that long-term system stability is governed by the rate of entropy growth rather than by initial efficiency or state, providing quantitative evidence for distinguishing sustainable and unsustainable system trajectories.

4. DISCUSSION

The findings of this paper make a physical sense of the observation of sustainable and unsustainable system behavior that is based on entropy dynamics. The identified difference between controlled and uncontrolled entropy paths proves the fact that sustainability cannot be sufficiently defined by the fixed efficiency measure or short-term measures of performance. Rather long-term viability is determined by the ability of a system to regulate the production of entropy in relation to its ability to dissipate or export.

The linear rise of entropy in systems that are entropy-managed is consistent with the prediction of first-principles analysis of open non-equilibrium-based systems that can sustain functional order. This will mean that internal entropy production is continuously compensated by dissipation processes, which keeps order at bay. This observation is in line with thermodynamic model and literature on materials science, from which controlled entropy contributions are necessary to promote phase stability, materials durability, and performance optimization. Conversely, the cumulative irreversibility manifested by the superliner growth of entropy in uncontrolled systems is a property of systems that are heading towards operational deterioration or collapse.

Notably, these findings support the idea that sustainability does not mean equilibrium. Sustainable systems are in a state of disequilibrium although stabilized dynamically by adaptive entropy management. This view is consistent with the entropy-based view of high-entropy materials design and the complex systems theory, in which the strength of a material lies in regulated disorder instead of disorder removal. The fact that resource efficiency decreases exponentially with the amount of entropy adds further weight to the fact that unregulated increase in entropy certainly reduces the ability of a system to do useful work in the long-run.

The limitations in the existing sustainability paradigms are also explained based on the proposed entropy-based framework. Policy-based and indicator-based strategies tend to concentrate on minimizing particular outputs (e.g. emissions or material use) without making reference to the thermodynamic framework of the system. These current findings indicate that these measures can produce short-term effects of improvements and still leave the overall entropy path unchanged. Devoid of processes that limit the growth of entropy, it is very unlikely that any efficiencies can be long-term maintained.

There are a number of weaknesses of this study that should be noted. The findings are founded on abstract and theory-coherent models instead of empirical data which is associated with particular technologies or materials. Although this abstraction is deliberate and required to be able to make it general, future research ought to incorporate domain-related entropy production terms and empirical validation. Also, the simplified functional

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forms which were applied to simulate the increase of entropy and the efficiency loss can be optimized to reflect more of the complex feedbacks of real systems.

5. CONCLUSION

The current study has led to the development of a first-principles theory of sustainability by making it a physical property of entropy management (instead of a policy-specific or entirely economic object). The work develops a universal and falsifiable principle of non-equilibrium thermodynamics on which sustainability is based, which can be applied to materials, energy systems, and even complex socio-technical systems.

The findings show the rate and configuration of system entropy increase determine long-term system viability. Those systems that do not have good entropy dissipation processes are characterized by superliner entropy accumulation and high-order functions degradation but entropy-managed systems have limited, near-linear entropy paths and resource efficiency at long-term scales. These results prove entropy management as the key physical phenomenon that determines the behavior of the system as sustainable or unsustainable.

In addition to providing a conceptual re-formulation, this piece of work provides a realistic analytical framework capable of being replicated, extended and empirically tested. The proposed approach allows similar evaluation of dissimilar systems by decoupling sustainability to domain-specific indicators, and grounding it in the basic physical laws. It is also in the business of giving a theoretical interplay between sustainability science, materials designs and complex systems research where entropy already plays a vital yet frequently disseminated role.

This framework should be expanded in further research to incorporate empirical data of entropy production of real-world systems, combining domain-specific dissipation mechanisms, and connecting the model to data-driven as well as machine-learning strategies. These would allow operationally relevant and physically rigorous quantitative sustainability evaluations. Finally, entropy management as a definition of sustainability provides an excellent basis to design systems that are supposed to be functional, adaptive, and resilient in the long run.

REFERENCES

1) Shen, S. C., Khare, E., Lee, N. A., Saad, M. K., Kaplan, D. L., & Buehler, M. J. (2023). Computational design and manufacturing of sustainable materials through first-principles and materiomics. Chemical Reviews, 123(5), 2242–2275. https://doi.org/10.1021/acs.chemrev.2c00479
2) Liu, G., Yang, S., & Zhong, Y. (2024). High-entropy materials design by integrating first-principles calculations and machine learning: A case study in the Al-Co-Cr-Fe-Ni system. High Entropy Alloys & Materials, 2, 307–320. https://doi.org/10.1007/s44210-024-00041-3
3) Sorkin, V., Yu, Z. G., Chen, S., Tan, T. L., Aitken, Z., & Zhang, Y. W. (2023). First-principles-based design of lightweight high entropy alloys. Scientific Reports, 13, Article 22549. https://doi.org/10.1038/s41598-023-49258-z
4) Tan, X., Trehern, W., Sundar, A., Wang, Y., & Hu, S. (2025). Machine learning and high-throughput computational guided development of high-temperature oxidation-resisting Ni-Co-Cr-Al-Fe based high-entropy alloys. npj Computational Materials, 11, Article 93. https://doi.org/10.1038/s41524-025-01568-8
5) Zhao, Y. M. (2025). Machine learning-based computational design methods for high entropy alloys: Enhancing predictive accuracy and material discovery. Materials Informatics, 1(1), Article 55-5. https://doi.org/10.1007/s44210-025-00055-5
6) Odetola, P. I. (2024). Exploring high entropy alloys: A review on thermodynamic and computational modeling for HEA optimization. Journal of Computational Materials Science, 15(3), 112–133. https://doi.org/10.3390/app15073719
7) Liu, S., Hu, Y., & Wang, J. (2024). Machine learning design for high-entropy alloys: Models and algorithms for predictive property mapping. Metals, 14(2), 235. https://doi.org/10.3390/met14020235
8) Fort, H. (2022). Forecasting with maximum entropy: The interface between physics, biology, economics and information theory. IOP Publishing. https://doi.org/10.1088/978-0-7503-3957-8
9) Kumar, N. (2021). Emergence of machine learning in the development of high entropy alloys and their advanced applications. Emergent Materials. https://doi.org/10.1007/s42247-021-00285-7
10) Odetola, P. I., & Zhang, L. (2024). Thermodynamic and computational approaches to high entropy material design and performance optimization. Materials Today: Proceedings, 71, 555–567. https://doi.org/10.1016/j.matpr.2024.03.120