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Research Article

Microscopic Interactions, Phase Stability, and Critical Phenomena in Condensed Matter Systems

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ABSTRACT

Condensed phases acquire their observable behaviour from interactions operating across several scales, from electronic charge redistribution and local bonding to collective order and thermodynamic stability. This paper develops an integrated theoretical and computational account of how microscopic interactions stabilize solid phases and how temperature, pressure, strain, and external fields can drive transitions between them. The analysis combines density-functional concepts, structural relaxation, energy and charge-density comparisons, statistical mechanics, molecular dynamics, Monte Carlo sampling, and free-energy modelling. Representative model outputs are used to demonstrate physically expected trends rather than to claim material-specific experimental measurements. Relaxed structures occupy total-energy minima; compression raises short-range electron-cloud repulsion, while expansion weakens bonding. Compact ordered phases consequently show stronger cohesion than distorted, layered, or disordered configurations at low temperature, although entropy and pressure can reverse their relative stability. Phase transformations are identified through free-energy crossings, abrupt or continuous structural changes, reduction of an order parameter, susceptibility enhancement, and movement of pressure-temperature boundaries. The combined results emphasize that local bonding alone is insufficient to describe a transition: collective fluctuations, entropy, finite-size effects, and competing configurations must also be considered. A practical predictive workflow is proposed in which candidate structures are optimized, competing energies are compared, thermodynamic corrections are introduced, atomistic or statistical sampling is performed, and the resulting phase boundary is validated. The framework provides a defensible basis for studying phase stability and critical phenomena while making clear the limitations of representative calculations and standard approximations.

Keywords: microscopic interactions; phase stability; critical phenomena; density functional theory; free energy; molecular dynamics; Monte Carlo simulation

1. Introduction

Condensed matter physics seeks to explain how a large number of closely interacting particles produce stable materials and collective phenomena. A solid is not simply an assembly of isolated atoms held at fixed coordinates. Its mechanical resistance, symmetry, thermal response, conductivity, magnetism, and capacity to transform into another phase emerge from the interaction of nuclei, electrons, lattice vibrations, and, in many systems, spin degrees of freedom. This many-body character is why two structures made from the same chemical elements can display sharply different macroscopic behaviour. Diamond and graphite are a familiar illustration: their contrasting properties follow from different bonding networks and dimensional arrangements rather than from a difference in elemental composition. The same principle extends to polymorphs, magnetic phases, pressure-induced structures, and ordered or disordered states.

The central problem addressed in this paper is the connection between microscopic stability and macroscopic phase transformation. At a microscopic level, atoms arrange themselves so that attractive interactions and short-range repulsion reach an energetic balance. Electron density may accumulate directionally between atoms, transfer from one species to another, or become delocalized over a metallic lattice. At a macroscopic level, however, the stable phase is determined not only by internal energy. Temperature introduces entropy, pressure introduces a volume contribution, and external fields can favour particular structural, electric, or magnetic arrangements. A structure that is the lowest-energy configuration at zero temperature may therefore cease to be stable when vibrational, configurational, or magnetic entropy becomes important.

The historical foundations of this analysis include crystallography, statistical mechanics, quantum mechanics, and critical-phenomena theory. X-ray diffraction established that crystalline materials possess ordered atomic arrangements (Bragg & Bragg, 1913). Quantum mechanical treatments later made it possible to interpret bonding and electronic energy in solids through many-electron theory and, practically, through density functional theory (Hohenberg & Kohn, 1964; Kohn & Sham, 1965). In parallel, the Ising model, Onsager's exact solution, scaling concepts, and renormalization-group approaches clarified how local interactions can create collective order and universal behaviour near critical points (Ising, 1925; Onsager, 1944; Kadanoff, 1966; Wilson, 1971a, 1971b). These lines of development show that phase behaviour must be studied through both microscopic energetics and statistical organization.

This paper reorganizes the source study into a focused research article with three aims. First, it examines how structural relaxation, bonding type, charge redistribution, cohesive energy, and spin exchange stabilize alternative condensed phases. Second, it analyses how phase changes are recognized through free energy, structural indicators, order parameters, susceptibility, and pressure-temperature boundaries. Third, it formulates a computational workflow for predicting phase stability while addressing convergence, finite-size effects, sampling, and model limitations. Because the underlying source presents representative theoretical outputs, the numerical values discussed here are treated as illustrative model results. Their purpose is to clarify interpretation and methodology, not to substitute for a complete material-specific dataset.

2. Microscopic and Thermodynamic Foundations

Phase stability begins with the competition between attractive and repulsive interactions. When atoms approach from large separation, bonding can lower the energy through orbital overlap, electrostatic attraction, or metallic electron delocalization. If the atoms are compressed too strongly, overlap of occupied electron clouds and nuclear repulsion raise the energy sharply. The equilibrium arrangement occurs near the minimum of the total-energy curve, where the net force on each atom is approximately zero. Structural relaxation is therefore more than a numerical procedure; it is the computational expression of the tendency of a condensed system to seek a mechanically stable configuration.

Different bonding mechanisms produce different structural signatures. Covalent bonds concentrate charge between particular atomic centres and often create short, directional connections. Ionic bonding involves charge transfer and electrostatic attraction, making coordination and local charge balance important. Metallic bonding spreads valence charge over many sites, which permits conductivity and often allows greater tolerance of deformation. Layered materials combine strong in-plane bonds with weaker interlayer attraction. Their anisotropy explains cleavage, exfoliation, directional transport, and the emergence of quasi-two-dimensional behaviour. In magnetic solids, exchange interactions add another stability channel because the total energy can depend on whether neighbouring moments are parallel, antiparallel, or disordered.

Cohesive energy and formation energy provide complementary measures of energetic preference. Cohesive energy compares the solid with isolated atoms, whereas formation energy compares a compound or phase with selected reference states. A more negative value generally

indicates stronger thermodynamic preference, but the choice of reference and the physical conditions must be stated. Importantly, the lowest-energy phase is not the only phase that may be observed. Metastable configurations can persist when a transformation requires nucleation, diffusion, or passage over a substantial energy barrier. Such phases are technologically valuable because they may offer electronic, optical, or mechanical properties absent from the ground state.

Thermodynamics expands this picture beyond static energy. At fixed temperature and pressure, a stable phase minimizes Gibbs free energy, $G = E + PV - TS$, where E is internal energy, P is pressure, V is volume, T is temperature, and S is entropy. At zero temperature and modest pressure, total-energy comparison can be adequate. At finite temperature, vibrational, configurational, electronic, and magnetic entropy may change the ordering of phases. Pressure favours structures with lower volume when the PV contribution offsets their internal-energy cost. Consequently, a dense phase that is unfavourable at ambient conditions may become stable under compression.

Order parameters connect thermodynamic stability with symmetry. Magnetization can distinguish an ordered ferromagnet from a paramagnet; sublattice displacement can measure structural symmetry breaking; density or a crystalline-order metric can separate ordered and disordered phases. In a continuous transition, the order parameter normally approaches zero smoothly. A first-order transition instead involves a discontinuity in a quantity such as volume, entropy, density, or magnetization and may show hysteresis. Binder (1987) emphasized the distinctive thermodynamics and finite-size signatures of first-order transitions, while Fisher (1967, 1998) and Wilson and Kogut (1974) developed the language of scaling and universality for continuous critical behaviour.

Susceptibility is especially informative near a critical point. In a magnetic model it is related to fluctuations of magnetization, while analogous response functions apply to structural or electronic order. A peak indicates that a small external perturbation can produce a large response. This enhancement arises because fluctuations become correlated over increasing distances: regions of spins, distortions, or density no longer fluctuate independently. Hohenberg and Halperin (1977) further showed that the dynamics of these fluctuations depend on conservation laws and coupling between slow variables. Thus, a phase transition is simultaneously an energetic, symmetry-related, and collective statistical event.

3. Computational Methodology

The research design combines analytical theory, first-principles modelling, atomistic simulation, and statistical sampling. Candidate systems include three-dimensional crystalline solids, layered structures, magnetic lattices, and idealized models such as Ising-type spin arrays. Initial structures are defined by lattice parameters, atomic coordinates, symmetry, and composition. Geometry optimization then relaxes atomic positions and, where appropriate, lattice dimensions until force and energy changes fall below chosen convergence thresholds.

Electronic energies and forces are obtained within a density-functional framework. The Hohenberg-Kohn formulation establishes the ground-state electron density as the central variable, and the Kohn-Sham equations transform the interacting problem into an effective one-particle problem (Hohenberg & Kohn, 1964; Kohn & Sham, 1965). A generalized-gradient approximation, such as the Perdew-Burke-Ernzerhof functional, provides a practical treatment of exchange and correlation for structural and energy trends (Perdew et al., 1996). Plane-wave calculations and iterative total-energy procedures are suitable for periodic solids (Kresse & Furthmüller, 1996). Energy cutoff, k-point sampling, supercell dimensions, relaxation criteria, and magnetic starting configurations must be tested before production calculations.

Microscopic interaction analysis uses bond lengths, coordination, lattice volume, charge-density difference, electron localization, cohesive energy, formation energy, and energy differences between magnetic configurations. Charge-density difference is interpreted by comparing the combined-system density with the densities of separated components. Accumulation between atoms supports covalent character, transfer between species supports ionic character, and broad delocalization supports metallic character. For magnetic models, exchange tendencies are inferred by comparing ferromagnetic, antiferromagnetic, and non-magnetic energies.

Phase-transition calculations vary temperature, pressure, strain, or field. Energy-volume data can be fitted to an equation of state, and enthalpy curves can be compared under pressure. A crossing identifies a candidate pressure-induced transformation. Temperature effects are treated with molecular dynamics, Monte Carlo simulation, or free-energy models. Molecular dynamics follows atomic motion and provides radial distribution functions, mean-square displacement, thermal expansion, and coordination changes. Monte Carlo sampling follows statistical acceptance rules, classically associated with the Metropolis algorithm, to explore equilibrium spin or configurational states (Metropolis et al., 1953).

Critical analysis tracks an order parameter, susceptibility, heat-capacity trend, correlation behaviour, and hysteresis. Simulations should be repeated for multiple cell sizes because finite systems can round transitions, suppress fluctuations, or enforce artificial periodic order. Heating and cooling paths help identify metastability and first-order hysteresis. Reliability is evaluated through convergence tests, repetition, comparison with accepted trends, and, when available, experimental or high-level theoretical benchmarks. The present study's numerical outputs are representative; therefore, the methodology supports qualitative interpretation and workflow design more strongly than exact material-specific prediction.

4. Results and Discussion

Structural relaxation produced the first consistent result: the equilibrium configuration lies near a minimum in relative total energy. Both compression and expansion increase energy, but for different microscopic reasons. Compression amplifies short-range repulsion between electron clouds and ions. Expansion reduces orbital overlap and weakens the attractive contribution to bonding. The minimum therefore represents the balance between these opposing effects. This outcome also provides an essential validation check; a supposedly optimized structure that does not occupy a local energy minimum cannot be treated as a stable phase.

Bond-length and coordination trends distinguish alternative phases. Compact structures have shorter average distances and higher coordination, while open or layered structures show larger volumes and greater anisotropy. A narrow bond-length distribution indicates a uniform crystal environment. A broadened distribution indicates local distortion, disorder, or thermal fluctuation. Small symmetry-breaking distortions may lower the energy relative to an ideal high-symmetry structure. Such a result is physically plausible because electronic degeneracy, magnetic ordering, strain, or lattice instability can make the symmetric configuration unstable.

Charge-density redistribution explains why geometry and stability change together. Directional accumulation between neighbouring centres produces strong but often brittle covalent networks. Charge transfer creates ionic stabilization and local dipoles that can influence dielectric and optical behaviour. Delocalized density screens ionic displacement and supports metallic flexibility. In layered phases, strong intralayer accumulation coexists with weak interlayer overlap. This combination stabilizes the sheet internally while permitting exfoliation and highly directional response. The analysis therefore supports a hierarchy:

electron redistribution determines bonding character, bonding determines structural organization, and structure influences the accessible phases.

Table 1. Representative energy-based stability comparison among model phases

Model phase	**Relative energy (eV/cell)**	**Cohesive trend**	**Interpretation**
Phase A: compact ordered solid	0.000	Highest magnitude	Reference stable phase at low temperature
Phase B: distorted crystalline phase	0.036	High; symmetry lowered	Metastable or strain-stabilized phase
Phase C: layered phase	0.092	Strong in-plane; weak interlayer	Favoured by reduced dimensionality or exfoliation
Phase D: disordered high-temperature phase	0.180	Reduced effective bonding	Can be stabilized by entropy at high temperature
Phase E: pressure-stabilized dense phase	-0.041 at high pressure	Enhanced packing stability	Favoured under compression

The representative energy comparison is summarized below. The values should be read as model indicators rather than measurements for a named compound.

At low temperature and ambient pressure, Phase A is the reference stable state because its compact, ordered network has the lowest baseline energy. Phase B is only 0.036 eV per cell higher, making it a plausible metastable or strain-selected structure. Phase C reflects a layered arrangement whose weaker interlayer cohesion raises its energy relative to a three-dimensional network but may still be favourable under reduced dimensionality or exfoliation. Phase D is energetically costly in a zero-temperature comparison, yet its disorder can provide an entropy advantage at high temperature. Phase E illustrates a pressure-stabilized dense phase: compression changes the thermodynamic balance sufficiently for it to become preferred.

Free-energy analysis converts these static comparisons into transition predictions. When the free-energy curves of two phases cross, the identity of the stable phase changes. Below the crossing, the lower curve defines the equilibrium phase; above it, the competing phase becomes favoured. The slope of each curve reflects entropy because S = -dG/dT at constant pressure. A phase with greater entropy can therefore overtake a lower-energy ordered phase as temperature rises. This explains why static zero-temperature energy alone cannot describe melting, order-disorder transformations, or high-temperature polymorphism.

Table 2. Phase-transition indicators and their physical meaning

Indicator	**Representative trend**	**Physical meaning**	**Likely interpretation**
Free-energy crossing	Two phase curves intersect	Identity of minimum-free-energy phase changes	Thermodynamic transition
Volume or density	Abrupt jump	Coexisting phases have different specific volumes	First-order transition
Order parameter	Gradual decrease to zero	Continuous loss of long-range order	Continuous transition
Susceptibility	Sharp peak near critical region	Strong response and correlated fluctuations	Critical phenomenon
Radial distribution	Long-range peaks weaken with temperature	Loss of crystalline order with surviving local order	Order-disorder or melting trend

Structural indicators separate continuous and discontinuous transformations. An abrupt jump in volume, density, coordination, or enthalpy supports first-order behaviour. Gradual reduction of a symmetry-breaking displacement supports a continuous transition. Radial distribution functions provide another diagnostic. Sharp peaks extending over long distance characterize crystalline order. Heating broadens these peaks, and a transition to a liquid or disordered phase removes long-range structure while frequently preserving a first-neighbour peak. Short-range order can therefore survive after translational order has disappeared.

The order-parameter result shows a progressive reduction of long-range order on approach to the critical temperature, followed by a zero or near-zero average above it. The accompanying susceptibility peak identifies a region of enhanced fluctuations. These two observables are complementary: the order parameter describes the mean degree of order, whereas susceptibility measures the scale of the response and its fluctuations. A transition should not be assigned from one noisy observable alone; agreement among energy, structure, order, and response strengthens the interpretation.

Pressure-temperature behaviour further demonstrates that a phase diagram is a multidimensional stability map. Pressure preferentially stabilizes dense structures through the PV term, but the most compressed geometry is not automatically stable because excessive compression raises repulsive energy. The stable high-pressure phase is the configuration that achieves the lowest combined internal-energy and volume contribution. An upward-sloping model boundary indicates that increasing pressure raises the temperature needed to destabilize the compact phase. This has practical significance: a material stable during room-condition characterization may transform during mechanical loading, thermal cycling, epitaxial strain, or field-driven operation.

A predictive model should therefore follow a staged workflow. First, candidate structures and magnetic arrangements are generated. Second, each configuration is relaxed and its energy, forces, bonding, and electronic state are checked. Third, competing phases are compared through energy, enthalpy, or free energy, depending on the variables of interest. Fourth, finite-temperature and configurational behaviour are introduced through phonons, molecular dynamics, Monte Carlo simulation, or Landau-type order-parameter models. Fifth, the phase boundary and response functions are tested for convergence, finite-size stability, and consistency with known physical limits.

Landau modelling is useful when the relevant symmetry and order parameter are known. Expanding free energy as a polynomial in the order parameter explains how an ordered minimum can appear below a critical temperature and disappear above it. The coefficients determine whether the change is continuous or first order. This approach does not replace atomistic calculation; instead, it organizes the transition in a compact phenomenological form and links microscopic results to measurable macroscopic behaviour.

Finite-size and sampling effects remain central limitations. A small supercell may suppress long-wavelength fluctuations, exaggerate order, or force periodic arrangements. A single

optimized configuration may miss competing defects, magnetic states, or disordered microstates. Near criticality, where fluctuations become large, these omissions can shift or blur the predicted transition. Repeating calculations across system sizes and initial conditions improves confidence. Likewise, heating and cooling trajectories reveal hysteresis and metastability that may be invisible in a single equilibrium scan.

Universality provides another level of interpretation. Materials with very different microscopic chemistry can display similar critical behaviour when they share dimensionality, order-parameter symmetry, and interaction range. Close to a continuous transition, the precise bond energy or atomic species may become less important than the way fluctuations scale with length. Critical exponents describe how the order parameter, susceptibility, heat capacity, and correlation length approach the transition. Kadanoff's block-scaling picture and Wilson's renormalization-group framework explain this loss of microscopic detail (Kadanoff, 1966; Wilson, 1971a, 1971b). For representative simulations, a simple peak or smooth curve is not enough to establish a universality class. One would need multiple system sizes, a well-defined reduced temperature, scaling collapse, and uncertainty estimates. Nevertheless, the framework identifies the correct observables and clarifies why finite-size analysis is scientifically important rather than a secondary computational refinement.

Thermodynamic preference must also be separated from transformation kinetics. Free-energy minimization predicts the equilibrium phase, but a real material may remain trapped in a metastable state because nucleation requires creation of an interface and collective atomic rearrangement. The barrier can depend on defects, grain boundaries, strain, diffusion, and heating rate. During a first-order transition, heating and cooling paths may therefore cross at different temperatures, producing hysteresis. Molecular dynamics can reveal rapid local restructuring but may not reach rare nucleation events within an accessible trajectory. Enhanced sampling, transition-path methods, or coarse-grained kinetic models may be needed when the mechanism and transformation rate are as important as the equilibrium boundary. This distinction prevents a common interpretive error: treating the phase with the lowest calculated free energy as though it must appear immediately in experiment.

Defects and interfaces can reshape the phase diagram even when their concentration is small. A vacancy changes local coordination and charge distribution; an impurity can donate carriers or create strain; an interface can impose lattice mismatch and break symmetry. These effects may stabilize a phase that is not preferred in the perfect bulk. Thin films are especially

sensitive because epitaxial constraint couples in-plane lattice parameters to structural distortion, while surfaces contribute a larger fraction of total energy. A bulk energy ranking should therefore not be transferred automatically to nanoparticles, coatings, heterostructures, or highly defective samples. The integrated workflow can be extended by comparing defect formation energies, interface energies, strained cells, and size-dependent free energies. Doing so would connect ideal phase theory with the conditions under which functional materials are actually synthesized and operated.

The same framework applies beyond purely structural transitions. In a magnetic transition, exchange energy competes with thermal disorder, magnetization serves as the order parameter, and susceptibility marks the region of strongest spin fluctuation. In a metal-insulator transition, the relevant change may involve carrier localization, orbital occupation, or a reconstruction of states at the Fermi level rather than a large displacement of atoms. Superconducting and quantum phase transitions introduce still different order parameters and may be driven by pressure, doping, field, or interaction strength at very low temperature (Vojta, 2003). These examples reinforce the need to choose observables according to the physical mechanism. A universal workflow does not mean using an identical calculation for every material; it means preserving the logic of candidate-state comparison, stability analysis, collective response, and validation while selecting the appropriate microscopic variables. For structural systems those variables include volume and coordination, for magnets they include spin correlations, and for electronic systems they include spectral weight and localization. This flexibility makes the approach useful across a broad range of condensed phases.

Uncertainty should be propagated through the workflow. Numerical convergence error, exchange-correlation choice, finite-size effects, uncertain entropy, and incomplete sampling all contribute to the final phase boundary. Reporting a single transition temperature with many significant figures can create false precision. A stronger practice is to calculate sensitivity to computational parameters, compare alternative functionals or interaction models, and present a stability interval where appropriate. If two phases differ by only a few tens of millielectronvolts per cell, methodological uncertainty may be comparable with the energy separation. In that situation, the scientifically defensible conclusion is that the phases are competitive and require higher-level theory or experimental discrimination, not that one phase is decisively stable.

The integrated results confirm that microscopic and collective descriptions are inseparable. Bonding and charge redistribution explain why a phase exists. Thermodynamics explains when that phase loses stability. Statistical mechanics explains the growth of correlated fluctuations. Pressure and field variables explain why the transformation boundary moves. The framework therefore avoids a common weakness in computational reporting: treating optimized geometry, energy curves, and transition plots as unrelated outputs. Their value lies in the causal chain connecting them.

5. Implications, Reliability, and Limitations

The framework has direct implications for material design. Metastable phases should not be dismissed simply because they are above the ground-state energy. Strain, interfaces, rapid cooling, pressure release, or kinetic barriers can preserve them, and their functional performance may exceed that of the equilibrium structure. Phase transitions themselves can serve as design mechanisms in sensors, switches, memory elements, and thermal-control devices when a modest external stimulus produces a useful change in structure, magnetization, or conductivity.

The reliability of any prediction depends on transparent computational practice. Structural parameters, cutoff energies, k-point meshes, cell sizes, magnetic configurations, thermostat or barostat choices, simulation length, and sampling procedures should be reported. The source methodology appropriately treats convergence and validation as part of the result rather than as hidden technical preparation. High-throughput databases and machine-learning models may accelerate discovery, but they remain dependent on the quality and physical relevance of their input data (Jain et al., 2013; Butler et al., 2018).

Experimental validation should be planned around the predicted mechanism. Diffraction can test symmetry and volume changes, calorimetry can detect latent heat or heat-capacity anomalies, spectroscopy can monitor electronic reconstruction, and magnetometry can follow a magnetic order parameter. High-pressure diffraction or transport can map compression-driven boundaries. Agreement across independent measurements is more persuasive than fitting one observable. Conversely, disagreement can reveal missing entropy, defects, kinetics, or correlation effects and should be used to improve the computational model rather than concealed as noise.

Several limitations restrict quantitative interpretation. Standard density-functional approximations may misrepresent strongly correlated states or delicate energy differences. Finite-temperature free energies require phonons, anharmonicity, magnetic entropy, or configurational entropy that are difficult to calculate fully. Molecular dynamics is restricted by accessible time and length scales, while Monte Carlo results depend on the chosen Hamiltonian and interaction parameters. Kinetic barriers can delay transformation even when thermodynamics favours another phase. These issues do not invalidate the integrated approach, but they require uncertainty to be acknowledged and exact transition temperatures to be validated against material-specific evidence.

6. Conclusion

This paper has shown that phase behaviour in condensed matter is produced by a connected sequence of microscopic, thermodynamic, and collective processes. Structural relaxation locates an energy minimum created by the balance of attraction and short-range repulsion. Charge redistribution, coordination, bonding directionality, electron delocalization, and spin exchange determine the relative stability of candidate structures. Cohesive and formation energies establish a zero-temperature baseline, while entropy, pressure, and external fields can reorder phase preference. Transitions are recognized most reliably through multiple indicators: free-energy or enthalpy crossings, structural discontinuities or gradual symmetry changes, order-parameter evolution, susceptibility enhancement, radial-distribution changes, and pressure-temperature boundaries. The representative results reproduce physically expected patterns, including low-temperature stability of compact ordered phases, entropy-driven competition from disordered phases, and pressure stabilization of dense structures. Their strongest contribution is methodological rather than material-specific. A defensible predictive workflow must combine optimized first-principles energies with thermodynamic modelling, atomistic or statistical sampling, finite-size tests, and validation. No single calculation is sufficient. By connecting electron density to bonding, bonding to structure, structure to free energy, and free energy to collective transformation, the framework provides a coherent basis for investigating phase stability and critical phenomena in advanced condensed matter systems.

References

Binder, K. (1987). Theory of first-order phase transitions. Reports on Progress in Physics, 50(7), 783-859. https://doi.org/10.1088/0034-4885/50/7/001

Bragg, W. H., & Bragg, W. L. (1913). The reflection of X-rays by crystals. Proceedings of the Royal Society A, 88(605), 428-438. https://doi.org/10.1098/rspa.1913.0040

Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O., & Walsh, A. (2018). Machine learning for molecular and materials science. Nature, 559, 547-555. https://doi.org/10.1038/s41586-018-0337-2

Fisher, M. E. (1967). The theory of equilibrium critical phenomena. Reports on Progress in Physics, 30(2), 615-730. https://doi.org/10.1088/0034-4885/30/2/306

Fisher, M. E. (1998). Renormalization group theory: Its basis and formulation in statistical physics. Reviews of Modern Physics, 70(2), 653-681. https://doi.org/10.1103/RevModPhys.70.653

Hohenberg, P. C., & Halperin, B. I. (1977). Theory of dynamic critical phenomena. Reviews of Modern Physics, 49(3), 435-479. https://doi.org/10.1103/RevModPhys.49.435

Hohenberg, P., & Kohn, W. (1964). Inhomogeneous electron gas. Physical Review, 136(3B), B864-B871. https://doi.org/10.1103/PhysRev.136.B864

Ising, E. (1925). Beitrag zur Theorie des Ferromagnetismus. Zeitschrift für Physik, 31, 253-258. https://doi.org/10.1007/BF02980577

Jain, A., Ong, S. P., Hautier, G., Chen, W., Richards, W. D., Dacek, S., Cholia, S., Gunter, D., Skinner, D., Ceder, G., & Persson, K. A. (2013). Commentary: The Materials Project. APL Materials, 1(1), 011002. https://doi.org/10.1063/1.4812323

Kadanoff, L. P. (1966). Scaling laws for Ising models near Tc. Physics Physique Fizika, 2(6), 263-272. https://doi.org/10.1103/PhysicsPhysiqueFizika.2.263

Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. Physical Review, 140(4A), A1133-A1138. https://doi.org/10.1103/PhysRev.140.A1133

Kresse, G., & Furthmüller, J. (1996). Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Physical Review B, 54(16), 11169-11186. https://doi.org/10.1103/PhysRevB.54.11169

Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., & Teller, E. (1953). Equation of state calculations by fast computing machines. The Journal of Chemical Physics, 21(6), 1087-1092. https://doi.org/10.1063/1.1699114

Onsager, L. (1944). Crystal statistics. I. A two-dimensional model with an order-disorder transition. Physical Review, 65(3-4), 117-149. https://doi.org/10.1103/PhysRev.65.117

Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. Physical Review Letters, 77(18), 3865-3868. https://doi.org/10.1103/PhysRevLett.77.3865

Vojta, M. (2003). Quantum phase transitions. Reports on Progress in Physics, 66(12), 2069-2110. https://doi.org/10.1088/0034-4885/66/12/R01

Wilson, K. G. (1971a). Renormalization group and critical phenomena. I. Renormalization group and the Kadanoff scaling picture. Physical Review B, 4(9), 3174-3183. https://doi.org/10.1103/PhysRevB.4.3174

Wilson, K. G. (1971b). Renormalization group and critical phenomena. II. Phase-space cell analysis of critical behavior. Physical Review B, 4(9), 3184-3205. https://doi.org/10.1103/PhysRevB.4.3184

Wilson, K. G., & Kogut, J. (1974). The renormalization group and the epsilon expansion. Physics Reports, 12(2), 75-199. https://doi.org/10.1016/0370-1573(74)90023-4

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