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Quantum Confinement and Coupled Electronic, Magnetic, and Optical Responses

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Abstract

Reducing a material from bulk dimensions to a sheet, wire, ribbon, or quantum dot changes the boundary conditions experienced by electrons and can reorganize its functional properties. This paper examines quantum confinement and the linked electronic, magnetic, and optical responses of low-dimensional condensed matter systems through a theoretical and computational framework. Band structures, density of states, wave-function localization, spin-polarized energies, spin density, dielectric response, and optical absorption are treated as mutually connected descriptors rather than isolated outputs. Representative model results show a progression from extended three-dimensional bands to subbands, sharp density-of-states features, localized edge or defect states, and discrete levels as dimensionality decreases. The electronic gap generally widens under stronger confinement, although edge states, defects, strain, and symmetry breaking can narrow the gap or introduce mid-gap levels. Magnetic moments can emerge when localized or spin-polarized states lower the energy, particularly at edges, defects, interfaces, or low-coordination sites. Optical absorption follows the available interband transitions and joint density of states; consequently, confinement may shift the absorption edge and sharpen spectral features, while structural distortion and defects can create red-shifted or sub-gap absorption. The paper proposes an integrated density-functional workflow with convergence tests appropriate to periodic and low-dimensional models, including vacuum separation, k-point sampling, supercell size, spin initialization, and cautious treatment of band gaps and excitonic effects. The main conclusion is that dimensional engineering changes the electronic spectrum and thereby changes magnetism and optical response. Reliable design of nanoscale materials must therefore connect structure, dimensionality, charge localization, spin order, and light-matter interaction within a single interpretive model.

1. Introduction

Low-dimensional materials occupy a central position in contemporary condensed matter physics because confinement changes the spectrum of allowed electronic states. A bulk crystal permits extended wave functions and energy dispersion in three spatial directions. A two-dimensional sheet confines motion in one direction; a nanowire confines motion in two; and a quantum dot confines carriers in all three. These changes are not merely geometric. They alter orbital overlap, screening, density of states, carrier localization, optical selection rules, and the stability of magnetic order. Consequently, a nanoscale system cannot be understood as a bulk crystal that has simply been made thinner.

The development of semiconductor nanocrystals and quantum dots established that size can tune optical and electronic behaviour (Alivisatos, 1996; Murray et al., 1993). The isolation of atomically thin carbon and the subsequent growth of graphene research demonstrated the distinctive physics of two-dimensional bands and quantum transport (Novoselov et al., 2004, 2005; Geim & Novoselov, 2007; Castro Neto et al., 2009). Transition-metal dichalcogenides then showed that reducing thickness can transform an indirect-gap bulk semiconductor into a direct-gap monolayer with strong photoluminescence (Mak et al., 2010; Splendiani et al., 2010). These developments established dimensionality as a design variable rather than a fixed material attribute.

This paper focuses on the causal relationship between quantum confinement and three major classes of measurable properties. Electronic behaviour is described through band dispersion, the position of the Fermi level, band-gap character, effective mass, and density of states. Magnetic behaviour is described through the energetic competition among spin configurations, local moment formation, exchange interaction, and spin-density distribution. Optical behaviour is described through the dielectric function, absorption onset, spectral peaks, reflectivity, and anisotropy. All three depend on the same underlying electronic states. Treating them separately can therefore produce an incomplete or even misleading assessment of material functionality.

The source study uses representative theoretical outputs covering bulk solids, two-dimensional sheets, one-dimensional structures, clusters, magnetic systems, semiconductors, and defective phases. This paper reorganizes those results into a focused research article. It asks four questions: How does reduced dimensionality reshape allowed energy states? Under what

conditions do localized states produce magnetic moments? How are optical transitions modified by confinement, distortion, and defects? What computational safeguards are required for credible low-dimensional calculations? The numerical trends are presented as illustrative models, not as experimental claims for a particular named material.

The analysis is also relevant to emerging quantum phases. Spin-orbit coupling and band inversion can produce topologically protected boundary states, while interfaces and moiré patterns can generate correlated or superconducting behaviour (Kane & Mele, 2005a, 2005b; Fu et al., 2007; Cao et al., 2018a, 2018b). Although the present representative framework does not calculate topological invariants or many-body excitations, it provides the band-structure, localization, and spin-resolved foundation from which such advanced studies can proceed.

2. Theoretical Background

Electronic states in a periodic solid arise when discrete atomic orbitals overlap and broaden into bands. Strong overlap generally creates wider bands and more dispersive carriers; weak overlap creates narrow bands and stronger localization. The valence-band maximum and conduction-band minimum determine the fundamental gap, while the presence of states at the Fermi level distinguishes a metal from a semiconductor or insulator. Density of states complements the band plot by counting the number of available states in each energy interval. Peaks can signal flat bands, van Hove singularities, localized orbitals, or reduced-dimensional subband structure.

Quantum confinement appears when a system dimension becomes comparable to the characteristic wavelength or spatial extent of the carrier state. Boundary conditions discretize momentum components and increase the separation between allowed energies. In a simplified picture, confinement energy scales inversely with the square of the confining length, so thinner structures tend to show larger level separation. Real materials complicate this trend through dielectric screening, strain, orbital rehybridization, surfaces, and many-body interactions, but the qualitative progression from bulk bands to discrete quantum-dot levels remains useful.

The shape of the density of states changes systematically with dimensionality. Three-dimensional systems often display comparatively smooth bands. Two-dimensional systems

develop step-like subband features. One-dimensional systems can produce sharp van Hove singularities. Zero-dimensional clusters exhibit discrete molecular-like levels. These changes affect carrier concentration, transport, magnetism, and optical absorption because they alter how many states are available near the Fermi level and at transition energies.

Surface, edge, and defect states are inseparable from low-dimensional physics. Atoms at a boundary have reduced coordination and may possess unsatisfied or reconstructed bonds. Their wave functions can localize spatially and introduce states inside or near the bulk gap. Such states may be beneficial, as in protected topological channels or engineered catalytic sites, or detrimental, as in non-radiative recombination centres. Anderson localization provides another route to spatial confinement when disorder prevents extended diffusion (Anderson, 1958). In practice, real low-dimensional materials combine geometric confinement with chemical edges, defects, substrates, and disorder.

Magnetism emerges when spin-polarized occupation lowers the total energy. A local moment requires an imbalance between spin-up and spin-down electrons, usually associated with partially filled or localized orbitals. Exchange interaction then determines how moments align across the structure. Low coordination and narrow bands can enhance localization and make magnetism more likely at edges or defects. Yet long-range order in an ideal isotropic one- or two-dimensional Heisenberg model is constrained at finite temperature by the Mermin-Wagner theorem (Mermin & Wagner, 1966). Real two-dimensional magnets evade this restriction through magnetic anisotropy, spin-orbit coupling, substrate effects, or discrete symmetry.

Optical response originates from transitions between occupied and unoccupied states. The imaginary part of the dielectric function describes absorptive transitions, while the real part describes dispersion and polarization. The absorption edge is related to the optical gap, and higher-energy peaks reflect the joint density of states and transition matrix elements. Confinement can shift the edge to higher energy and sharpen features. However, excitonic binding becomes stronger when screening is reduced, particularly in two-dimensional systems. Standard independent-particle calculations may therefore underestimate the complexity of measured optical spectra, and many-body approaches such as GW and the Bethe-Salpeter equation are needed for quantitative quasiparticle gaps and excitons.

Topology introduces a distinct form of boundary physics. In topological insulators and related systems, edge or surface states are protected by symmetry and global properties of the electronic wave functions rather than by ordinary dangling bonds (Hasan & Kane, 2010; Qi & Zhang, 2011; Chiu et al., 2016). Band inversion, spin-orbit coupling, Berry curvature, and topological invariants must be evaluated to establish such phases. The present framework treats localized boundary states more generally, while recognizing that topological analysis is an important extension.

3. Computational Methodology

The computational design begins with structural models representing bulk, monolayer or thin-film, nanoribbon or nanowire, and finite cluster geometries. Bulk crystals use periodic boundary conditions in three dimensions. Sheets use periodicity in two directions with vacuum normal to the layer. Wires use periodicity along one axis with vacuum in the other two, while finite clusters require a sufficiently large non-periodic cell. Vacuum separation must be tested because interaction between periodic images can create artificial dispersion, charge transfer, or magnetic coupling.

Ground-state electronic structure is treated through density functional theory based on the Hohenberg-Kohn and Kohn-Sham formulations (Hohenberg & Kohn, 1964; Kohn & Sham, 1965). Plane-wave or equivalent periodic basis methods are suitable for crystalline and layered systems, and a generalized-gradient functional such as PBE provides a practical starting point for geometry and qualitative band trends (Perdew et al., 1996; Kresse & Furthmüller, 1996). More advanced hybrid, GW, or correlated methods may be required when exact gaps, quasiparticle levels, or strong electronic correlation are central.

Each structure is relaxed before property calculation. Atomic positions, and sometimes lattice parameters, are optimized until residual forces and total-energy changes satisfy selected criteria. The analysis records bond lengths, symmetry, layer thickness, edge reconstruction, and local coordination. Convergence tests cover plane-wave cutoff, k-point density, supercell length, vacuum thickness, and, for metallic or narrow-gap systems, electronic smearing. A low-dimensional calculation that omits vacuum or supercell convergence risks reporting artifacts as physical confinement.

Electronic analysis includes band structure along appropriate high-symmetry paths, total and projected density of states, Fermi-level position, orbital character, and charge or wave-function localization. The band gap is identified from the valence-band maximum and conduction-band minimum, with attention to whether the transition is direct or indirect. Projected states reveal which atoms and orbitals form the band edges. Spatial plots determine whether edge, surface, or defect levels are extended or localized.

Magnetic calculations require multiple starting configurations. Ferromagnetic, antiferromagnetic, ferrimagnetic, and non-magnetic arrangements are compared rather than assuming a single spin state. The lowest converged total energy identifies the preferred configuration within the chosen approximation. Local moments and spin-density maps show where magnetization resides. If exchange parameters are extracted, statistical spin models can estimate thermal ordering trends, but such temperatures are sensitive to cell size, anisotropy, and the mapping procedure.

Optical response is calculated from transitions between occupied and unoccupied states. The dielectric function, absorption coefficient, refractive index, and reflectivity can be derived within an independent-particle approximation. Direction-resolved calculations are essential for anisotropic sheets and wires. A denser k-point mesh and sufficient unoccupied bands are normally required for smooth spectra. Interpretation links each absorption feature to band-edge orbitals, density-of-states peaks, and allowed transition channels.

Validation is qualitative in the representative source study. Expected trends include gap widening with stronger confinement, sharper low-dimensional density-of-states features, finite Fermi-level states in metals, spin localization at selected sites, and absorption onsets compatible with the calculated band structure. Exact numerical values would require material-specific structures, reported convergence data, advanced corrections, and comparison with experiment.

4. Results and Discussion

The representative band-structure result displays a semiconducting separation between occupied valence states and unoccupied conduction states. This basic outcome illustrates how the periodic potential transforms atomic levels into bands and forbidden energy intervals. If a band

crossed the Fermi level, the phase would be metallic; if the separation were substantially larger, it would behave as an insulator. The moderate gap of the model semiconductor is therefore a starting point for assessing how dimensionality, strain, defects, and magnetic order modify functionality.

The density of states confirms the band classification. A low or vanishing density at the Fermi level is consistent with a semiconductor or insulator, whereas a finite density indicates a metal. Peaks identify energies with many available states. Projected density of states is particularly important because it connects spectral features to orbital chemistry. For example, a transition-metal d orbital may create narrow states near the Fermi level and support magnetism, while more dispersive s or p states may dominate conduction and optical transitions.

Dimensional reduction produces the trend summarized below.

Table 1. Representative dimensionality-dependent electronic-state trends

Dimensionality	**Electronic-state feature**	**Expected gap trend**	**Physical interpretation**
Three-dimensional bulk	Continuous dispersion in three directions	Smallest or reference gap	Weak confinement; extended wave functions
Two-dimensional sheet	Subbands and strong surface sensitivity	Moderate increase	Out-of-plane confinement and anisotropy
One-dimensional nanowire	Sharp van Hove-like DOS features	Larger increase	Radial confinement and channel transport
Zero-dimensional dot or cluster	Discrete molecular-like levels	Largest level separation	Full spatial confinement
Defective low-dimensional system	Localized edge or defect levels	May narrow or create mid-gap states	Under-coordination changes allowed states

Note. Trends are representative and can be reversed or modified by strain, chemistry, reconstruction, dielectric screening, and charge transfer.

The table captures the central confinement sequence. Bulk states remain extended and disperse in all directions. A two-dimensional sheet loses out-of-plane dispersion and develops stronger anisotropy. A one-dimensional wire confines carriers radially and produces sharper density-of-states structures. A quantum dot replaces continuous bands with discrete levels. Defects and edges complicate this sequence by creating localized states that can narrow the apparent gap or insert levels inside it.

Gap widening under confinement follows from increased kinetic energy and greater level separation, but it is not universal. Structural relaxation can change bond lengths and orbital hybridization. Edge termination can introduce occupied or empty boundary states. Strain may shift the relative energies of valleys or orbitals. Charge transfer from a substrate can move the Fermi level. Accordingly, a credible confinement study must compare geometries after relaxation and explain the band change in terms of orbital contribution and localization, not simply report a numerical gap.

Wave-function plots distinguish extended and localized states. In the bulk model, band-edge states spread through the lattice. In a sheet, the wave function is confined normal to the plane but remains extended in-plane. In a nanoribbon, certain states may accumulate at zigzag or armchair edges depending on chemistry and symmetry. A defect-rich model can show intense localization around a vacancy or substituted atom. Such localization increases scattering and can reduce carrier mobility, yet it may also create active states for sensing, catalysis, or magnetism.

The magnetic analysis compares spin-polarized configurations through total energy. A stable magnetic state requires the spin-polarized solution to be lower in energy than the non-magnetic alternative and to retain physically meaningful local moments after convergence. Ferromagnetic order corresponds to parallel moments, while antiferromagnetic order corresponds to alternating moments with little or no net magnetization. Ferrimagnetism combines opposing unequal moments. In low-dimensional systems, edge states or narrow defect bands can satisfy the conditions for local moment formation because localization increases the energetic importance of exchange.

Spin density provides the spatial explanation. A moment concentrated on a defect indicates localized magnetism; distribution over several sites indicates more itinerant or exchange-coupled

behaviour. Interfaces can modify moment size through charge transfer, hybridization, and symmetry breaking, which is why interface-induced magnetism is a major design route (Hellman et al., 2017). Antiferromagnetic and spin-orbit phenomena are also relevant to spintronics because electrical currents can manipulate spin order without requiring a large net magnetization (Baltz et al., 2018; Manchon et al., 2019).

The optical spectrum begins near the first allowed interband transition and develops peaks where the joint density of occupied and unoccupied states is large and the transition matrix element is non-zero. A confinement-widened gap can move the onset to higher photon energy, producing a blue shift. Reduced dimensionality also sharpens density-of-states features, which can sharpen optical peaks. Conversely, symmetry breaking or defect levels can produce a red-shifted edge or sub-gap absorption. These trends link optical response directly to the electronic structure rather than treating absorption as an independent material characteristic.

Table 2. Integrated electronic, magnetic, and optical interpretation

Phase type	**Electronic behaviour**	**Magnetic response**	**Optical implication**
Compact semiconductor	Moderate clean band gap	Weak unless spin centres exist	Defined absorption edge
Distorted phase	Reduced gap from symmetry breaking	Possible enhanced local moment	Red-shifted absorption
Metallic phase	Finite DOS at Fermi level	Possible itinerant polarization	Free-carrier response and high reflectivity
Low-dimensional phase	Confinement-driven gap change	Edge magnetism may appear	Sharper, anisotropic absorption
Defect-rich phase	Mid-gap states and Fermi-level shift	Localized defect moments	Sub-gap absorption or recombination pathways

Note. Functional value depends on balancing structural stability, carrier transport, spin order, and optical transition strength.

The integrated property summary shows why a single descriptor is insufficient. A compact semiconductor may be structurally stable and possess a clean gap, yet it may have weak absorption in the desired spectral region. A distorted phase may absorb more strongly because symmetry breaking reduces the gap, but it can also be less stable. A metallic phase supports free-carrier response and high reflectivity but may not provide useful interband emission. A low-dimensional phase can display a widened gap and sharper absorption, while edge states may introduce magnetism. A defect-rich phase may be useful for sub-gap detection but may also suffer rapid carrier recombination.

Anisotropy is one of the most important low-dimensional outcomes. In-plane orbitals often overlap more strongly than out-of-plane orbitals, creating direction-dependent effective masses, conductivity, dielectric response, and absorption. Optical spectra should therefore be reported for multiple polarization directions. A single averaged curve can hide the property most relevant to a device. The same principle applies to transport and magnetism, where easy-axis anisotropy can determine whether two-dimensional order survives at finite temperature.

The results also indicate several control strategies. Thickness engineering changes confinement strength. Strain modifies bond lengths, symmetry, and orbital overlap. Doping and gating move the Fermi level and can populate magnetic or conducting states. Edge functionalization passivates or deliberately creates boundary levels. Defects can be introduced to generate local moments or sensing sites. Heterostructures combine layers with different band alignment, screening, and spin-orbit coupling. Each strategy acts first on the electronic structure and only then on the observable magnetic or optical property.

Topological and correlated phases represent advanced extensions of the same logic. Spin-orbit coupling can invert bands and produce protected edge states in suitable symmetry classes (Kane & Mele, 2005a, 2005b; Fu et al., 2007). Twisted two-dimensional layers can flatten bands, enhance interactions, and generate correlated insulating or superconducting states (Cao et al., 2018a, 2018b). These phenomena require calculations beyond the present representative workflow, including Berry curvature, topological invariants, many-body correlation, or large moiré supercells. Nevertheless, careful band, orbital, localization, and spin analysis remains the necessary starting point.

Confinement also changes carrier effective mass and transport anisotropy. A strongly dispersive band corresponds to a relatively small effective mass and usually supports higher mobility, whereas a flat band corresponds to heavier, more localized carriers. When a bulk crystal becomes a sheet or ribbon, the curvature of the band can change differently along each direction. The resulting material may conduct readily along one axis but poorly along another. This effect is especially important in nanoribbons, where edge orientation can alter band dispersion and scattering. Therefore, a gap value by itself does not establish device quality. A useful channel material must combine an appropriate gap with favourable band curvature, stable contacts, manageable defect scattering, and an electrostatically controllable carrier density.

The distinction between direct and indirect gaps is equally important. In a direct-gap semiconductor, the valence-band maximum and conduction-band minimum occur at the same crystal momentum, allowing efficient optical transitions without phonon assistance. In an indirect-gap material, momentum conservation normally requires a phonon, reducing radiative efficiency. Thickness can reorder valleys and convert an indirect bulk material into a direct-gap monolayer, as demonstrated for MoS2 (Mak et al., 2010; Splendiani et al., 2010). A computational comparison should therefore track both the magnitude and momentum location of the band edges. Optical usefulness depends further on symmetry and polarization selection rules; an energetically allowed transition may remain weak if its matrix element is small.

Reduced dielectric screening strengthens electron-hole attraction. The optical excitation energy can then lie substantially below the quasiparticle band gap because the excited electron and remaining hole form a bound exciton. This effect is often pronounced in two-dimensional semiconductors, where electric field lines extend into the surrounding environment. Substrate dielectric constant, encapsulation, layer number, and carrier density can consequently shift exciton binding and optical peaks without greatly changing the underlying atomic structure. Independent-particle spectra are valuable for identifying orbital transitions and qualitative anisotropy, but they should not be equated automatically with measured absorption or photoluminescence. Quantitative treatment requires quasiparticle corrections and an electron-hole interaction calculation, commonly through GW and the Bethe-Salpeter equation.

Temperature and environment can further modify low-dimensional properties. Lattice vibrations broaden electronic levels, shift gaps, and scatter carriers, while thermal expansion

changes orbital overlap. A free-standing monolayer may ripple, and a supported layer may inherit strain, screening, or charge from its substrate. Adsorbed molecules and ambient oxidation can alter edge states and local moments. Consequently, a zero-temperature calculation on an ideal isolated sheet represents a controlled reference, not the complete operating material. Ab initio molecular dynamics, electron-phonon calculations, explicit substrate models, and disorder averaging are natural extensions. Comparing these results with spectroscopy, transport, microscopy, and magnetometry would determine whether a predicted state remains robust under realistic conditions. This step is essential for moving from attractive computational descriptors to reproducible device performance.

Functional optimization involves trade-offs. Strong localization can create magnetic moments and intense optical transitions, yet it can also reduce mobility and increase non-radiative recombination. A wide confinement-induced gap can improve transistor switching but shift absorption away from the visible spectrum. Defects can enable sub-gap sensing while degrading stability. Heavy elements can provide spin-orbit coupling for topological or spintronic behaviour but may introduce toxicity, cost, or fabrication challenges. The most promising material is therefore not necessarily the one with the largest gap, moment, or absorption peak. It is the one whose combined structural stability, electronic dispersion, magnetic robustness, optical response, and environmental compatibility match a specific application.

The principal interpretive result is that dimensionality modifies a shared electronic foundation. Confinement changes dispersion and density of states. Those changes affect localization and exchange, which determine magnetic tendencies. The same occupied and unoccupied states determine optical transitions. Therefore, electronic, magnetic, and optical outputs should be evaluated together. A report that lists a band gap, magnetic moment, and absorption peak without tracing their common orbital origin misses the physical mechanism and weakens predictive value.

5. Applications, Reliability, and Limitations

The coupled framework supports material design for transistors, photodetectors, light-emitting devices, solar-energy conversion, magnetic memory, spin logic, sensors, and quantum technologies. Semiconducting sheets with tunable gaps are attractive for flexible electronics and optoelectronics. Localized magnetic edge states may support spin filters or nanoscale memory.

Strong anisotropic absorption can be exploited in polarization-sensitive detectors. Topological boundary states offer possible low-dissipation channels, while magnetic skyrmions and spin-orbit torques provide alternative information carriers (Nagaosa & Tokura, 2013; Fert et al., 2017).

Reliability requires low-dimensional checks that are sometimes unnecessary in bulk work. Vacuum separation, dipole correction, layer number, edge termination, supercell size, defect concentration, and substrate representation can all change the answer. Multiple magnetic initial states are essential because self-consistent calculations can become trapped in metastable solutions. Band-gap underestimation should be acknowledged, and optical spectra based on independent particles should not be presented as fully excitonic predictions.

Experimental comparison should likewise be property-specific. Photoemission and tunnelling spectroscopy probe band dispersion and density of states; optical absorption and photoluminescence probe excitations; scanning probes reveal local defects and edge states; transport measures mobility and carrier type; and magnetic microscopy or magnetometry tests spin order. Because each technique samples different aspects of the electronic system, apparent discrepancies may be physically meaningful. A strong validation strategy aligns the calculated observable with the measurement and uses multiple techniques to separate intrinsic confinement from substrate, defect, and environmental effects.

The representative source results are qualitative. They reproduce expected relationships but do not identify a single compound, synthesis route, measured transition, or experimentally verified device. Strong correlation, spin-orbit coupling, excitons, electron-phonon effects, disorder, temperature, and environmental screening may require methods beyond standard ground-state density functional theory. For quantitative comparison, future work should use material-specific structures, quasiparticle corrections, Bethe-Salpeter optical calculations, finite-temperature dynamics, and experimental validation.

6. Conclusion

Quantum confinement changes condensed matter by changing the permitted electronic states. As dimensionality is reduced from bulk to sheet, wire, and dot, dispersion becomes restricted, density-of-states features sharpen, and energy levels become increasingly discrete. The

fundamental gap often widens, but the final electronic structure also depends on relaxation, strain, chemistry, defects, edges, substrates, and charge transfer.

Magnetic and optical behaviour follow from these same states. Localized or narrow bands can produce spin polarization and local moments, especially at low-coordination boundaries or defects. Optical absorption is controlled by the occupied and unoccupied spectrum, transition matrix elements, and dielectric screening; confinement can blue-shift and sharpen features, while defects or distortion can create red-shifted and sub-gap response. Directional bonding further produces strong anisotropy in transport and light-matter interaction.

The central methodological conclusion is that band structure, density of states, wave-function localization, spin density, and optical spectra must be interpreted as one connected dataset. Credible predictions also require vacuum and supercell convergence, multiple magnetic configurations, cautious treatment of band gaps, and recognition of excitonic and many-body limitations. By linking dimensional structure to electronic spectrum and then to magnetic and optical function, the framework provides a coherent foundation for designing low-dimensional and quantum materials.

References

Alivisatos, A. P. (1996). Semiconductor clusters, nanocrystals, and quantum dots. Science, 271(5251), 933-937. https://doi.org/10.1126/science.271.5251.933

Anderson, P. W. (1958). Absence of diffusion in certain random lattices. Physical Review, 109(5), 1492-1505. https://doi.org/10.1103/PhysRev.109.1492

Baltz, V., Manchon, A., Tsoi, M., Moriyama, T., Ono, T., & Tserkovnyak, Y. (2018). Antiferromagnetic spintronics. Reviews of Modern Physics, 90(1), 015005. https://doi.org/10.1103/RevModPhys.90.015005

Cao, Y., Fatemi, V., Demir, A., Fang, S., Tomarken, S. L., Luo, J. Y., Sanchez-Yamagishi, J. D., Watanabe, K., Taniguchi, T., Kaxiras, E., Ashoori, R. C., & Jarillo-Herrero, P. (2018a). Correlated insulator behaviour at half-filling in magic-angle graphene superlattices. Nature, 556, 80-84. https://doi.org/10.1038/nature26154

Cao, Y., Fatemi, V., Fang, S., Watanabe, K., Taniguchi, T., Kaxiras, E., & Jarillo-Herrero, P. (2018b). Unconventional superconductivity in magic-angle graphene superlattices. Nature, 556, 43-50. https://doi.org/10.1038/nature26160

Castro Neto, A. H., Guinea, F., Peres, N. M. R., Novoselov, K. S., & Geim, A. K. (2009). The electronic properties of graphene. Reviews of Modern Physics, 81(1), 109-162. https://doi.org/10.1103/RevModPhys.81.109

Chiu, C.-K., Teo, J. C. Y., Schnyder, A. P., & Ryu, S. (2016). Classification of topological quantum matter with symmetries. Reviews of Modern Physics, 88(3), 035005. https://doi.org/10.1103/RevModPhys.88.035005

Fert, A., Reyren, N., & Cros, V. (2017). Magnetic skyrmions: Advances in physics and potential applications. Nature Reviews Materials, 2, 17031. https://doi.org/10.1038/natrevmats.2017.31

Fu, L., Kane, C. L., & Mele, E. J. (2007). Topological insulators in three dimensions. Physical Review Letters, 98(10), 106803. https://doi.org/10.1103/PhysRevLett.98.106803

Geim, A. K., & Novoselov, K. S. (2007). The rise of graphene. Nature Materials, 6, 183-191. https://doi.org/10.1038/nmat1849

Hasan, M. Z., & Kane, C. L. (2010). Colloquium: Topological insulators. Reviews of Modern Physics, 82(4), 3045-3067. https://doi.org/10.1103/RevModPhys.82.3045

Hellman, F., Hoffmann, A., Tserkovnyak, Y., Beach, G. S. D., Fullerton, E. E., Leighton, C., MacDonald, A. H., Ralph, D. C., Arena, D. A., Dürr, H. A., Fischer, P., Grollier, J., Heremans, J. P., Jungwirth, T., Kimel, A. V., Koopmans, B., Krivorotov, I. N., May, S. J., Petford-Long, A. K., et al. (2017). Interface-induced phenomena in magnetism. Reviews of Modern Physics, 89(2), 025006. https://doi.org/10.1103/RevModPhys.89.025006

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

Kane, C. L., & Mele, E. J. (2005a). Quantum spin Hall effect in graphene. Physical Review Letters, 95(22), 226801. https://doi.org/10.1103/PhysRevLett.95.226801

Kane, C. L., & Mele, E. J. (2005b). Z2 topological order and the quantum spin Hall effect. Physical Review Letters, 95(14), 146802. https://doi.org/10.1103/PhysRevLett.95.146802

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

Mak, K. F., Lee, C., Hone, J., Shan, J., & Heinz, T. F. (2010). Atomically thin MoS2: A new direct-gap semiconductor. Physical Review Letters, 105(13), 136805. https://doi.org/10.1103/PhysRevLett.105.136805

Manchon, A., Zelezny, J., Miron, I. M., Jungwirth, T., Sinova, J., Thiaville, A., Garello, K., & Gambardella, P. (2019). Current-induced spin-orbit torques in ferromagnetic and antiferromagnetic systems. Reviews of Modern Physics, 91(3), 035004. https://doi.org/10.1103/RevModPhys.91.035004

Mermin, N. D., & Wagner, H. (1966). Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models. Physical Review Letters, 17(22), 1133-1136. https://doi.org/10.1103/PhysRevLett.17.1133

Murray, C. B., Norris, D. J., & Bawendi, M. G. (1993). Synthesis and characterization of nearly monodisperse CdE semiconductor nanocrystallites. Journal of the American Chemical Society, 115(19), 8706-8715. https://doi.org/10.1021/ja00072a025

Nagaosa, N., & Tokura, Y. (2013). Topological properties and dynamics of magnetic skyrmions. Nature Nanotechnology, 8, 899-911. https://doi.org/10.1038/nnano.2013.243

Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y., Dubonos, S. V., Grigorieva, I. V., & Firsov, A. A. (2004). Electric field effect in atomically thin carbon films. Science, 306(5696), 666-669. https://doi.org/10.1126/science.1102896

Novoselov, K. S., Jiang, D., Schedin, F., Booth, T. J., Khotkevich, V. V., Morozov, S. V., & Geim, A. K. (2005). Two-dimensional atomic crystals. Proceedings of the National Academy of Sciences, 102(30), 10451-10453. https://doi.org/10.1073/pnas.0502848102

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

Qi, X.-L., & Zhang, S.-C. (2011). Topological insulators and superconductors. Reviews of Modern Physics, 83(4), 1057-1110. https://doi.org/10.1103/RevModPhys.83.1057

Splendiani, A., Sun, L., Zhang, Y., Li, T., Kim, J., Chim, C.-Y., Galli, G., & Wang, F. (2010). Emerging photoluminescence in monolayer MoS2. Nano Letters, 10(4), 1271-1275. https://doi.org/10.1021/nl903868w