Quantum Matter: Topology and Correlations driving new materials, phases, and phenomena

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Abstract. I review the classification of quantum matter as a function of Coulomb interactions $U$ and spin-orbit coupling $\lambda$ in units of the bandwidth. The region where all three of these energy scales are comparable, as in the 4d and 5d transition metal oxides and dichalcogenides is the most promising for discovering new materials and new phenomena. I discuss what it means to extract a model from a material and the hierarchy of computational methods for single and multi-orbital systems. As specific examples I describe half metallic high-$T_c$ ferromagnetism in the double perovskite $\text{Sr}_2\text{FeMoO}_6$ in which the kinetic energy of Mo ($d^5$) electrons drives ferromagnetic exchange between the Fe ($d^5$) core spins. I will also discuss predictions for materials with a $d^4$ electronic configuration with strong spin-orbit coupling and show that there is a large parameter space where instead of a $J=0$ band insulator one surprisingly finds ground states with orbitally entangled ferromagnetic states. I will conclude with a broad outlook for new discoveries in this arena.

1. Introduction

It is evident that over the past decades, the discovery, understanding and applications of new solid-state materials have played a crucial role in modern technology. However, devices today based on silicon have hit a bottleneck in terms of the amount of information that can be packed in nano-dimensions and still avoid the complications due to heating [1]. For the design of the next generation of multifunctional devices, we need new paradigms, new principles and new classes of materials. The question then arises: which specific materials do we investigate? In this review article, we start by giving a big picture for guiding exploration of novel materials and then focus on two stories that highlight half metallic conduction in a high-$T_c$ ferromagnet and novel ferromagnetism in strongly spin-orbit coupled systems.

If we classify quantum matter in the plane described by spin-orbit coupling (SOC) $\lambda$ and Coulomb correlations $U$ relative to the bandwidth $W$ (Figure 1), we have the traditional metals and insulators at weak $U$ and $\lambda$ shown in the bottom left quadrant. These would include metals such as aluminum, insulators such as silicon that have ruled our electronics applications, and the newly emerging semimetal graphene with Dirac linear dispersion [2-3]. At large $U$, in the bottom right quadrant, are the transition metal oxides with partially filled $3d$ shells that have dominated materials research in the past.
decades, leading to such spectacular phenomena as high-$T_c$ superconductivity [4-5] and colossal magnetoresistance (CMR) [6-7]. Even though high $T_c$ superconductivity in the cuprate family was discovered almost 25 years ago the problem still remains unsolved. This is because strong correlations make density functional theory (DFT) approaches inapplicable and theoretical predictions unreliable, making the feedback loop between theory and experiments difficult. Once electrons interact strongly and correlations dominate, the movement of one electron requires the adjustment of all the other electrons and the electronic structure, which is essentially a map of how a single electron behaves in a solid, becomes an inadequate description of the problem. From a materials point of view, oxides are notorious for problems of segregation and inhomogeneity across various length scales such that controlling the composition and homogeneity of oxides over entire range of carrier concentration is highly challenging.

It is important to note that for multi-orbital systems, we are simplifying the situation by denoting the interactions by a single parameter $U$ which should more realistically be broken down into intra-orbital and inter-orbital (Hund’s) interactions. However, for the present discussion a single $U$ axis suffices to bring out the qualitative aspects of the discussion. Continuing on, in the large $\lambda$ - small $U$ quadrant (Figure 1 top left) we have the prediction [8-10] and subsequent detection [11-12] of topological band insulators (TBI) in s- and p- band materials. The topological properties of these materials are best preserved in the absence of broken time reversal symmetry. One of the primary difficulties in developing useful applications based on TBI has been the inability to pin the chemical potential within
the band gap which not only mixes signals from the topological surface states and the bulk bands in measuring their properties but is also a hindrance for many applications.

The uncharted territory for new materials and new physics is in the middle involving 4d and 5d transition metals where all energy scales, $W$, $U$, and $\lambda$, are comparable as emphasized in Figure 2. We expect new phases and new phenomena to emerge from the close interplay of these energy scales. In this context the transition metal oxides (TMO) [13-16] and transition metal dichalcogenides (TMDCs) [17-19] with comparable correlations, SOC and bandwidth $W$, are emerging as the dream materials both in terms of their fundamental properties and potential applications [20]. The TMDCs have layered structures similar to graphene that makes them easier to grow compared to the oxide based materials. In addition they can have considerably richer properties compared to graphene given both the tunable SOC and correlations. Both of the classes of materials, the TMO and TMDC materials with heavy transition metal atoms and with moderate correlations have the potential to combine the properties of the second (top left) and fourth (bottom right) quadrants shown in Figures 1 and 2. They bring together the advantages of topologically-protected surface states arising from the large SOC, as well as the magnetism from correlations. There is the potential for using strain to modulate the orbitals and through that the magnetism via the spin-orbit coupling. Given their moderate correlations, they are theoretically much more tractable and allow for a quick iterative cycle between experiment and theory.

2. Hierarchy of computational complexity and extracting a meaningful model

The first step in modelling a material is to use the known atoms and crystal structure and obtain the electronic structure using density functional theory (DFT). At the next level of complexity we can enhance the tightbinding electronic structure by including spin orbit coupling. From this we can often extract a tightbinding Hamiltonian by a downfolding procedure focusing on a few target bands. For example, in the case of graphene, we can obtain a tightbinding Hamiltonian with a single orbital on a
honeycomb lattice that describes the electronic structure at low energies near the chemical potential. Density functional methods include Coulomb correlations within an effective one-electron picture. Several packages are available for calculating the electronic structure given the types of atoms and the crystal structure [21]. The topological properties must be elucidated by a topological band analysis of the associated wave functions [22-24]. Once correlations are included, even in a single orbital model, the complexity increases enormously. At the simplest level we obtain a one-band Hubbard model [25]. To treat the onsite interaction [Eq. (2)], one approach is to embed a single site or a cluster of sites in a fermionic bath and solve the problem self-consistently, known as dynamical mean field theory (DMFT). The “dynamical” in DMFT indicates that quantum fluctuations, even though at the level of a single site or a cluster of sites, are included [26]. Even the solution of the single site problem requires quantum Monte Carlo (QMC) methods [27,28] for its solution, though other solvers using exact diagonalization and perturbation theory are also prevalent. There has been recent progress in solving the impurity model by using the hybridization expansion version of the continuous time quantum Monte Carlo (CT-HYB) [29] implemented in the TRIQS code [30] for rotationally invariant interaction using conserved quantities to speed up the calculations.

Single site DMFT largely avoids the sign problem, which is one of its great virtues. The sign problem however begins to appear in more sophisticated versions like cluster DMFT or in dynamical cluster approximation (DCA), and also in real space approaches like determinantal quantum Monte Carlo (DQMC). There are however difficulties of going to low temperatures because of the fermion sign problem and accessing the superconducting state and difficulties of obtaining the real frequency spectral function and density of states even at higher temperatures in the pseudogap region because of uncertainties associated with analytic continuation.

![Diagram of a honeycomb lattice and a model](image)

**Figure 4:** Using Picasso “bull” pictures to illustrate the successive extraction of the model in the context of graphene. Graphene is a honeycomb lattice of carbon atoms; each C consists of a filled helium core plus 4 valence electrons $2s^2 2p^2$ occupying $(s, p_x, p_y, p_z)$ orbitals. The honeycomb lattice is represented as a triangular lattice with 2 atoms in the unit cell i.e. with 8 electrons and 8 orbitals in the unit cell. As the unit cells are brought together to make a solid, the orbitals overlap and form 8 bands. In general, C also has unoccupied d-orbitals that form bands. This electronic structure is the “higher level” model for graphene. At the next level of simplification, if the physics we are considering is only sensitive to states close to the Fermi energy, we can extract a tight-binding model with a single band. This band is primarily of $p_z$ character, with some mixing of other orbitals. We obtain an excellent fit to the actual single band with a single hopping parameter $t=2.64$ eV. If necessary the quality of the fit can be improved with additional hopping parameters. Now if one is interested in physics on the scale of few 100 meV then it is possible to focus on just the linear dispersion near the Dirac points and simplify the Hamiltonian to $H = \pm v_F \vec{\sigma} \cdot \vec{p}$. This brings out the beauty of graphene, its topological nature, the presence of two Dirac points with linear dispersion at K and K’ in the Brillouin zone with opposite Berry curvature.
As discussed above, there has been considerable progress using dynamical mean field theory and its cluster-based generalizations, which however still requires DQMC for the solution of the impurity or cluster problem as well as maximum entropy methods for extracting dynamical information. It is important in this context to bring up complementary variational methods that are based on a wave function and are constructed by using some intuition for the phenomenon being proposed. The variational estimate provides an upper bound to the energy and can be creatively used to get information about moments of spectral functions. Most importantly, because the absolute square of the wave function is sampled, they do not suffer from the sign problem. In the context of the Hubbard model, projected wave functions have provided understanding about the origin of two energy scales, a pairing scale vs. a coherence scale, with completely different doping dependencies, and the broadening of the spectral function with underdoping [31,32].

As we move into the uncharted territory of 4d and 5d transition metal oxides and dichalcogenides, we must include the complexity of multi-orbitals, the crystal field splittings, the intra- and inter-orbital correlations and spin-orbital coupling. How do we begin to make sense of such complexity? Clearly, the problem must first be investigated using simple test cases with exact diagonalization, effective models and simple mean field theory first to build understanding and identify directions followed by multi-orbital generalizations of DMFT thereby paving the way for a full QMC analysis.

Iterated cycle between theory, computation and experiments: Several conceptual steps are necessary to go from a material to a model as best illustrated by Picasso [33] in his sketches of the “bull” going sequentially from a realistic rendition (“the material”) to a simplified sketch capturing the bare essentials (“the model”). The degree of simplification can depend on the questions that are being explored. In other words there need not be a single model for a given material but depending on the nature of the questions, for example, whether charge degrees are important or spin, the range of energies being explored and other factors one can have a series of models. This too is best illustrated by Picasso’s bull pictures shown below in the context of graphene in Figures 4. To summarize then, the first step in modeling a new material is to start with the known elements and structure and obtain the full electronic structure from first principles DFT methods to identify the important orbitals. This can be followed by an ab initio downfolding procedure to obtain an effective low energy tight-binding Hamiltonian, with further reduction toward an effective magnetic Hamiltonian. The effective Hamiltonians can then be used to calculate phase diagrams, identifying phases and their transport and dynamical susceptibilities using mean field theory and QMC methods.

Interplay of Spin-Charge-Orbital degrees (Fig 5 top): In half-filled electronic systems, strong Coulomb correlations U can open a Mott gap in the density of states. By favoring single occupancy of electrons on a site, the strong U also leads to the formation of local moments. The low energy sector is dominated by spin interactions that typically gives rise to antiferromagnetic ground states in half filled systems but also competing ferromagnetic interactions based on Goodenough-Kanamori rules in multi-orbital systems. In the presence of spin-orbit coupling acting in the e_s or t_{2g} sectors, the resulting magnetic interactions become directional, and can lead to Mott-assisted insulators. A new tuning knob now emerges—lattice strain—which can manipulate the orbitals and thereby the spin degrees.
We can see the vast panorama of possibilities in material synthesis and design that is available by tuning SOC and interaction parameters (both intra-orbital and inter-orbital), lattice structure and the valency of the transition metal ion. In order to keep the rest of the discussion somewhat focused, we next demonstrate such a multi-pronged theoretical and computational approach applied to two problems based on the double perovskite structure.

**3A. Perovskites with half metallicity and high-Tc Ferrimagnetism**

Sr$_2$FeMoO$_6$ (SFMO) is an important example of a material that exhibits a fully polarized metallic ground state and a ferromagnetic T$_c$ of around 425K [34-36]. This combination of properties has the potential for an enormous technological impact in spintronic applications such as tunneling magnetoresistance devices. What is the fundamental mechanism underlying such behavior? In SFMO Fe$^{3+}$ is in a 3$d^5$ electronic configuration and because of the large Hund’s coupling the five electrons completely fill the $d\uparrow$ orbitals and behave as an $S=5/2$ core spin. Mo$^{5+}$ is in a 4$d^1$ electronic configuration. This Mo electron in the $t_{2g}$ orbital could be either up or down in principle. However, it
chooses to be down because the electron can gain kinetic energy by delocalizing via the Fe $d_{\downarrow}$ orbitals that are empty. In addition to previous mean field theories [37-40] we use exact diagonalization (ED) to solve the quantum mechanics of “fast” itinerant electrons moving in the background of “slow” $S=5/2$ spins, for which we use a $T \neq 0$ classical Monte Carlo (MC) simulation [41-43].

Using standard ED-MC techniques, supplemented by $T=0$ variational calculations, we obtain the results shown in Figs. 7 and 8. We show in Fig. 7 the band structure and the spin-resolved density of states (DOS) $N_{\sigma}(E)$ for the ferromagnetic ground state of SFMO with $n=0.33$ electrons per unit cell per plane. These results are consistent with photoemission experiments [44]. We consider three different characterizations of magnetization: the core Fe spin magnetization, the itinerant Mo spin magnetization and the itinerant spin polarization at the Fermi surface. We find that the conduction electrons, with magnetization $M_{el}(T=0)=1\mu_B$ (per unit cell), are polarized opposite to the Fe spins, with core spin magnetization $M_S(0)=5\mu_B$. The half-metallic ground state, with $N_{\uparrow}(0) \neq 0$ and $N_{\downarrow}(0)=0$, has a net magnetization $M(0)=M_S(0)-M_{el}(0)=4\mu_B$. We see from Fig. 8 that $M_S(T), M_{el}(T)$ and hence the total magnetization $M(T)=M_S(T)+M_{el}(T)$ all have essentially the same $T$ dependence. Another quantity of great interest is the conduction electron polarization $P(T)$ at $E_f$ which determines the tunneling magnetoresistance. This is defined below:

Figure 6: (top) The quantum itinerant Mo electron moving in the fluctuating magnetic field of the Fe core spins treated classically. (bottom) The spin-resolved (red: $\downarrow$; blue $\uparrow$) electronic structure of the Mo electron and the density of states found to be strongly temperature dependent from half metallic at $T=0$ to unpolarized above $T_c$. 

![Diagram](image_url)
Effective Spin Hamiltonian: The results of Fig. 8 imply that the core spin magnetization $M_s(T)$ and the electronic polarization $P(T)$ are linked. This is an important observation, since the former is much easier to measure. With this motivation, we derive an effective Hamiltonian $H_{\text{eff}}$ for the core spins by generalizing the two-site Anderson-Hasegawa [45] analysis for manganites to double perovskites. To derive $H_{\text{eff}}$, we find the exact solution of the full $H$ for one electron in two unit cells. The Hilbert space has three states per unit cell: Fe $t_{2g}$ and Mo $t_{2g}$, leading to a 6 x 6 matrix for two unit cells.

We analytically find its lowest eigenvalue as a function of the angle $(\theta_i - \theta_j)$ between core spins and find the nearest-neighbor ($J_1$) and next-nearest-neighbor ($J_2$) interaction energies; see the inset in Fig. 8(b). Expressing these in terms of $S_i \cdot S_j$ where each $S_j$ is a unit vector, we obtain the effective circles), and (3) the Heisenberg model as a test case (blue dashes). These results are obtained on 8 systems with error bars no larger than the symbol size. (d) Magnetization $M(T)$ from 3D simulations of $H_{\text{eff}}$ on 16 systems; $T_c$ is obtained by from finite scaling

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P(T) = \frac{N_i(0) - N_i(0)}{N_i(0) + N_i(0)}\] measured at $E_f$. In Fig. 8, we also see that $P(T)$ follows the $M_s(T)$.

Figure 7: The core spin magnetization, $M_s(T)$, conduction electron magnetization $M_{\text{el}}(T)$ and polarization $P(T)$ at $E_f$ calculated using a combination of exact diagonalization for the itinerant electrons moving in a spin texture of the core electrons obtained by classical Monte Carlo.

(b) Spin-wave dispersion of the full Hamiltonian $H$, obtained by exact diagonalization, compared with that of the effective Hamiltonian $H_{\text{eff}}$. Inset: Fe-Mo lattice showing the nearest-neighbor $J_1$ and next nearest-neighbor $J_2$ interactions between Fe-Fe ions described by $H_{\text{eff}}$. (c) The normalized magnetization for three Hamiltonians: (1) the exact $H$ with itinerant spins moving in a background of fluctuating core spins (black squares), (2) the effective magnetic Hamiltonian for double perovskites (red
Hamiltonian

\[ H_{\text{eff}} = -J_1 \sum_{\langle i,j \rangle} F_1(S_i \cdot S_j) - J_2 \sum_{\langle i,j \rangle} F_2(S_i \cdot S_j) \]

where the functions

\[ F_1(x) = 8(2 + \sqrt{2} + 2x) \quad \text{and} \quad F_2(x) = (5 + \sqrt{5})\sqrt{6 + 2\sqrt{3} + 2x}. \]

Our two-unit cell analysis gives explicit expressions for \( J_1 \) and \( J_2 \), both of which are ferromagnetic, with their scale set by the kinetic energy \( t \) of delocalization. We emphasize that the double square-root form of \( H_{\text{eff}} \) is quite different from the (single square-root) Anderson-Hasegawa model. Next, we need to understand how we can use \( H_{\text{eff}} \) going beyond the simple two-unit cell derivation. Specifically:

(i) how can we relate \( J_1 \) and \( J_2 \) to \( t, t', \Delta \) and the filling?

(ii) To what extent does \( H_{\text{eff}} \) capture the essential physics of the full Hamiltonian \( H \)? To validate the effective model \( H_{\text{eff}} \), we show in Figure 8 that it reproduces the magnetization \( M(T) \) of the full Hamiltonian \( H \) over the entire range of temperatures. In contrast, the Heisenberg model \( H_{\text{Heis}} \) gives quite different results, except in the \( T \rightarrow 0 \) limit with small spin deviations.

Thus, we cannot describe the \( M(T) \) for the DP’s using a Heisenberg model, while \( H_{\text{eff}} \) provides an excellent description of the ED-MC result.

The classical \( H_{\text{eff}} \) can be easily simulated on large 3D lattices, unlike the full \( H \), and the results are shown in Fig. 8. We note the linear drop in \( M(T) \) at low \( T \), due to classical spin waves, followed by a rapid suppression of \( M \) at the phase transition. Our \( M(T) \) results are in qualitative agreement with recent experiments [46]. We estimate \( T_c \) in the infinite volume limit using the finite size scaling of results obtained on \( L^3 \) systems with \( L = 8, 12, 16 \). For \( t'/t = 0.1 \) and \( \Delta/t = 2.5 \) we find \( T_c = 0.14t \).

Comparing this to \( T_c^{\text{exp}} = 420 \) K for pure SFMO, we obtain \( t = 0.27 \) eV consistent with Ref. [36].

3B: Novel Ferromagnetism in \( d^4 \) electronic configuration

The interplay of strong interactions and spin-orbit coupling (SOC) naturally combines in the 5d transition metal materials, which hold the potential for hosting new phases of matter with entangled...
spin, orbital and charge degrees of freedom. Already there are many predictions for exotic topological matter, for example the topological Mott insulators and Weyl semi-metals. Recent experiments demonstrating that Sr$_2$IrO$_4$ is an unusual Mott insulator with a half filled $j=1/2$ band resulting from strong SOC [47] have prompted the search for Weyl semi-metals in iridium pyrochlores [48]. We emphasize that most of the focus in this field to date has been on iridium based materials with a $d^5$ electronic configuration. In the limit of strong spin orbit coupling the $t_{2g}$ orbitals are split into $j=1/2$ and $j=3/2$ multiplets. For the $d^5$ configuration, all of the $j=3/2$ states are filled and the only low-energy degree of freedom is a single hole in the $j=1/2$ manifold which is sufficient to understand most phenomena. This picture is often given in terms of non-interacting atomic levels, but it also holds in the strongly interacting limit for the $d^5$ configuration.

The physics is dramatically different for other fillings. Mott insulators with $d^1$ and $d^2$ configuration have been shown to exhibit exotic magnetic states [49, 50] in the presence of large SOC. In the $d^1$ case, SOC is quenched in a cubic environment [51] and the problem reduces to a conventional spin-only model. This leaves only the $d^4$ case, which has been largely ignored because it is expected that large SOC and strong interactions give rise to a non-magnetic state in the atomic limit [49], though see [52]. We show [53] that, contrary to the above expectation, the $d^4$ configuration has a rich magnetic phase diagram as a function of SOC and Hubbard $U$. In particular, at large $U$ there is a quantum phase transition from the expected non-magnetic insulator of local $J=0$ singlets to a ferromagnetic insulator with a nonzero local moment as SOC is reduced. This moment arises from super-exchange induced mixing, at a single site, of magnetic states largely from the higher energy triplet with the singlet. Our result provides an interesting counterexample to the commonly held notion that Mott insulators have well defined local moments that cannot be affected by small perturbations (compared to the interaction scale $U$).

To begin, we perform exact diagonalization on a two-site system with minimal assumptions. From here we can extract the effective magnetic Hamiltonian and then generalize to a lattice. The lattice problem can then be analyzed by various methods such as mean field theory and variational methods. For the two-site problem the number of states required for exact diagonalization are 12 choose 8 which is approximately 500 states arising from the 3 ($t_{2g}$ orbitals) x 2 (sites) x 2 (spin) and 8 electrons. As a function of $\lambda$ and $U$ there are three different magnetic states as shown in Figure 9: (i) a non-magnetic state $J=0$ in the large $\lambda$ limit, (ii) a ferromagnet with $J=2$ for small $\lambda$ and moderate $U$, and (iii) a ferromagnet with $J=1$ at large values of $U$ and small $\lambda$. The magnetic phases can be understood easily in limiting cases. The $J=0$ state at large $\lambda$ and small $U$ corresponds to a band insulator with a completely filled $j=3/2$ manifold. The post-perovskite material NaIrO$_3$ and perovskites BaOsO$_3$ and CaOsO$_3$ are believed to be in such a state [54,55,56]. With increasing $U$, this band insulator smoothly crosses over into a $J=0$ Mott insulator (as defined by real-space localization of charge, and a single-particle excitation gap set by the large interaction energy scale). In the limit of small $\lambda$ and moderate $U$, the $J=2$ ferromagnet is essentially the Stoner ferromagnet seen in SrRuO$_3$. The most interesting phase is the $J=1$ ferromagnet at large $U$ and small $\lambda$, which has been often overlooked because the naive atomic limit analysis predicts a nonmagnetic insulator. However, its existence can be understood as follows. For large $U$, each site $i$ has a well defined $|L_i|=1$ and $|S_i|=1$. The superexchange interaction is ferromagnetic because of Hund’s coupling, and that therefore stabilizes the total $S=2$ state for the two-site problem. The total orbital moment is however not maximized and a total $L=1$ state is realized; upon including SOC in the $L-S$ coupling scheme yields the observed $J=1$ state. In sharp contrast, an atomic limit analysis gives $J_i=0$ singlet states at each site in accordance with Hund’s third rule with the caveat that $L_i=-1$ for $t_{2g}$ orbitals.

We propose candidate materials from the double perovskite family, with cubic crystal field, which can be tuned across the magnetic transition by chemical substitution and/or pressure. In the double
perovskite $\text{A}_2\text{BB}'\text{O}_6$ where $\text{A}$ is an alkaline earth element while $\text{B}$ and $\text{B}'$ are two different transition metal ions, ordered in a 3D checkerboard pattern, if we choose the $\text{B}$ sites to have completely filled shells, the bandwidth is suppressed, giving rise to a Mott insulator. When combined with a 4d or a 5d element on the $\text{B}'$ site, we have the ideal model system where large SOC competes with ferromagnetic exchange. Of particular interest is $\text{La}_2\text{ZnRuO}_6$ which is an insulator with Ru in the d$^4$ configuration. Two different samples grown by two different groups have shown very different magnetic states. One group has found a ferromagnetic state with $T_c=165$K [57], while the other found a non-magnetic state [58]. We believe $\text{La}_2\text{ZnRuO}_6$ is very close to the phase boundary and small differences in the lattice parameter may be the origin of this discrepancy. A resonant x-ray scattering study under pressure will be an ideal experiment to observe the phase transition. Another closely related material is $\text{La}_2\text{MgRuO}_6$ [57], which is also a promising candidate.

4. Conclusions
At this stage we are just beginning to scratch the problem of multiorbitals with intra (Hubbard $U$) and inter (Hund’s) orbital interactions and spin-orbit coupling $\lambda$. We expect to see the growth of paradigmatic multi-orbital Hamiltonians and effective magnetic Hamiltonians with directional interactions that harbor non-trivial magnetic Mott insulators and metallic states. With the corresponding materials growth from the transition metal oxide and dichalcogenide families, we expect to see a rich dialog between theory and experiment.

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