A materials informatics approach to the identification of one-band correlated materials analogous to the cuprates

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One important yet exceedingly rare property of the cuprate high-temperature superconductors is the presence of a single correlated $d$ band in the low-energy spectrum, leading to the one-band Hubbard model as the minimal description. In order to search for materials with interesting strong correlation physics as well as possible benchmark systems for the one-band Hubbard model, here we present a new approach to find one-band correlated materials analogous to the cuprates by leveraging the emerging area of materials informatics. Using the composition, structure, and formation energy of more than half a million real and hypothetical inorganic crystalline materials in the Open Quantum Materials Database, we search for synthesizable materials whose nominal transition metal $d$ electron count and crystal field are compatible with achieving an isolated half-filled $d$ band. Five Cu compounds, including bromide, oxide, selenate, and pyrophosphate chemistries, are shown to successfully achieve the one-band electronic structure based on density functional theory band structure calculations. Further calculations including magnetism and explicit on-site Coulomb interaction reveal significant evidence for strong correlation physics in the five candidates, including Mott insulating behavior and antiferromagnetism. The success of our data-driven approach to discovering new correlated materials opens up new avenues to design and discover materials with rare electronic properties.

I. INTRODUCTION

The cuprates, one of the most famous classes of materials in condensed matter physics, are layered copper-oxide ceramics with copper-oxygen planes exhibiting unconventional, high-temperature superconductivity. Despite decades of study, the details of the mechanism and phase diagram of this class of materials is still not fully settled, due in part to a complex phase diagram in which doping the antiferromagnetic Mott insulating parent compound leads to pseudogap, charge density wave, spin density wave, and “strange metal” phases in addition to the superconducting phase. However, it is generally accepted that the presence of a single $d$ orbital at low energy is a very important characteristic leading to the high critical temperature $T_c$ for superconductivity in the cuprates.

A minimal model for the physics of the cuprates is the one-band Hubbard model (1BHM) corresponding to the Hamiltonian

$$\hat{H}_{1BHM} = -t \sum_{i,j,\sigma} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}.$$ 

Here $\hat{c}_{i\sigma}^{\dagger}$ annihilates (creates) an electron of spin projection $\sigma$ on lattice site $i$, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$, $t$ is the hopping parameter, and the on-site Coulomb repulsion $U$ parametrizes the strength of the electronic correlations. Although the 1BHM is easy to write down, this many-body Hamiltonian has only been solved in one (using the Bethe ansatz) and infinite (using dynamical mean-field theory) dimensions. In general, $t$ leads to delocalized electronic states and metallic behavior, whereas $U$ localizes the electrons. In correlated materials like the parent compounds of the cuprates, $U$ is large with respect to $t$ and (Mott) insulating behavior is found.

Thus, the cuprates can be considered correlated one-band materials. We are not aware of any correlated one-band material outside of the cuprates. One key reason for their rarity is that most transition metal compounds have octahedral or tetrahedral coordination, for which the $5d$ orbitals split into a group of 3 ($T_g$ for octahedral) and a group of 2 ($E_g$ for octahedral) according to group theory. Therefore, while a multiband Hubbard model is considered to be achieved in many compounds, realizations of the 1BHM are very rare. The discovery of such materials would be highly desirable for two purposes:

1. To search for new unconventional superconductors or materials exhibiting other interesting strong correlation phenomena, and
2. To provide physical realizations of the 1BHM to serve as benchmarks for our theories of strong correlation physics.

Recent efforts to achieve such a material have not been successful. For example, Chaloupka and Khaliullin proposed to break the symmetry of the $E_g$ levels in octahedral LaNiO$_3$ by forming a superlattice with LaAlO$_3$. Unfortunately, the experiments suggest that this approach yields insufficient symmetry breaking to achieve a one-band model. LiCuF$_3$ and related compounds were proposed in the trigonal bipyramidal coordination, whose symmetry does lead to a singly-degenerate level. Although it was shown to have promising characteristics, LiCuF$_3$ is not thermodynamically stable under ambient conditions.

Here we employ the emerging area of materials informatics to accelerate the search for one-band correlated materials analogous to the cuprates. In order to identify candidate materials, we devise a materials...
database search strategy based on (1) the elements contained in the material, (2) the local coordination geometry of atoms in the crystal structure, (3) nominal valence electron count for each element, and (4) thermodynamic stability. In particular, we look for (1) compounds containing transition metals and anions, (2) transition metals coordinated by anions in a coordination environment whose crystal field leads to a singly-degenerate $d$ level, (3) transition metals with a nominal $d$ electron count leading to half filling of such a level, and (4) compounds that are thermodynamically stable or nearly stable. For example, the cuprate parent compound La$_2$CuO$_4$ would satisfy criteria (2) and (3) since Cu is in a square planar environment and nominally in a $d^9$ configuration, half-filling a singly-degenerate $B_{1g}$ ($d_{x^2−y^2}$) level. We query for any crystal that simultaneously satisfies all four criteria. We execute our strategy using the Open Quantum Materials Database (OQMD), an extensive electronic structure database with calculations for over 550,000 real and hypothetical inorganic crystalline materials (as of June 2017).

We successfully identify five correlated one-band materials: CuBr$_2$, Li$_2$CuO$_2$, BaCu(SeO$_3$)$_2$, SrCu(SeO$_3$)$_2$, and K$_3$H(CuP$_2$O$_7$)$_2$. DFT calculations incorporating corrections for electronic correlations demonstrate promising characteristics in these materials including antiferromagnetism and Mott insulating behavior. Additionally, our findings illustrate the power of high-throughput computing and materials informatics to search for complex materials possessing rare electronic properties.

II. METHODOLOGY

A. Screening strategy

Our materials informatics screening approach consists of several materials properties that must be simultaneously satisfied:

1. **Chemistry** – Compound must contain transition metal and anion elements, and (for practicality) no radioactive elements

2. **Crystal structure** – In the compound, transition metals (TMs) must be in a coordination whose local symmetry yields one or more singly-degenerate $d$ orbitals based on crystal field theory. The coordinations considered are linear, trigonal planar, square planar, trigonal bipyramidal, square pyramidal, trigonal prismatic, pentagonal bipyramidal, and square antiprismatic.

3. **Electron count** – All TM in the compound must have a nominal $d$ electron count corresponding to a half-filled singly-degenerate level given the crystal field splitting of the coordination environment.

4. **Thermodynamics** – The compound must be no more than 25 meV/atom above the thermodynamic ground state (as determined via convex hull analysis) and/or reported experimentally. This criterion is designed to focus on compounds which are likely to be synthesizable. The particular threshold value of 25 meV/atom is chosen to match the magnitude of computed hull distances for synthesized metastable compounds found by Sun et al. for most chemistries.

Our search strategy is executed on the OQMD an open database containing calculations of over half a million known and hypothetical inorganic crystalline compounds derived from the Inorganic Crystal Structure Database (ICSD) and structural prototypes. The OQMD contains electronic structure calculations at the DFT level and in some cases DFT+$U$ level at consistent sets of parameters to enable consistent thermodynamic analysis.

We include details on the coordination environments considered in this study in the Supplemental Material. A description of our method for nominal electron counting and for the local structural queries performed to ascertain coordination environments are included in our previous work. The coordination environment query relies on separate computation (outside of the qmpy framework) of the TM nearest-neighbor bond lengths and angles, which are not directly stored in the OQMD.

Our screening strategy only requires computation of the electronic band structure as a post-processing step for a small number of candidate materials. An alternative approach of directly analyzing the electronic band structures that exist in materials database is not applicable for our purpose primarily because such databases only contain band structures already including spin polarization and Hubbard $U$ effects, rather than the underlying non-spin-polarized DFT band structure. This is problematic since the desired isolated band, if present, can be hidden once it is spin-split and pushed into other bands, as in the case of VS$_2$. We use the projector augmented wave method, a 600 eV kinetic energy cutoff, and uniform $k$-point meshes of $k$-point density of 350/Å$^{-3}$ or greater. The ionic forces and total energy are converged to 0.001 eV/Å and 10$^{-6}$ eV, respectively. The high-symmetry $k$-point paths for band structures are based on the AFLOW conventions.
III. RESULTS AND DISCUSSION

A. High-throughput materials screening

We begin by discussing the number of materials obtained via our high-throughput materials screening strategy. Figure 1 illustrates how the number of candidate compounds is reduced from the total as successive filtering criteria are applied. Note that a logarithmic scale is used since many orders of magnitude are spanned. Removing compounds containing radioactive elements eliminates 120,000 compounds from the total of 550,000 candidates. We next filter by stability by including only compounds which are thermodynamically stable or nearly stable (no more than 25 meV/atom above the ground state). Irrespective of the computed stability, we also keep any compound if it has been reported experimentally. 43,000 compounds remain after this filter. 18,000 of the 43,000 contain a TM and an anion and 4,000 of these have a $d$ electron count compatible with one or more of the desired local coordination environments. Finally, we find that 187 of the compounds contain the corresponding coordination environment.

The two biggest decreases (in a fractional sense) of candidate compounds are (1) the stability filter, in which the number of compounds is reduced from 430,000 to 43,000 and (2) the local structure filter, in which the number is reduced from 4,000 to just 187. The substantial decrease in candidate compounds from the stability filter, a general observation not tied specifically to searching for one-band correlated materials, is reflective of the high percentage of unstable, hypothetical compounds in the OQMD derived from structural prototypes. The significant decrease in candidates from the structural screening criterion reflects the infrequency of the low-symmetry coordination environments that lead to singly-degenerate $d$

![FIG. 1. Materials database screening for correlated one-band materials. Decrease in the number of compounds, on a logarithmic scale, as additional screening criteria are applied from left to right.](image1)

B. Distribution of structure, chemistry, and thermodynamic stability

We now describe the 187 candidate compounds identified by our screening strategy. The distribution of local TM coordinations for the 187 candidate compounds are displayed in Fig. 2(a). Square planar coordination is the most common, with nearly 50% of the total. Trigonal prismatic and linear coordinations are also found in significant numbers. Some of the more obscure coordinations like pentagonal bipyramidal are not found in a single compound.

![FIG. 2. Characterization of the identified compounds. Distribution of the 187 candidate compounds in terms of (a) TM coordination geometry, (b) thermodynamic stability, and (c) identity of the TM and its nearest-neighbor element.](image2)
ICSD prototypes are trigonal planar La₃CuSiS₂-type (7, e.g. Sm₃CuSnSe₇), trigonal prismatic NbS₂-type (5, e.g. TaSe₂), linear CaTiO₃-type (5, e.g. InCo₃N), and square planar Ca₂CuCl₂O₂-type (5, e.g. Sr₂CoBr₂O₃).

The only six hypothetical compounds derived from structural prototypes rather than the ICSD are CsWO₃, HfBr₃, Mn₂TeO, BiPd₃, Ni₃Sb, and Zr₃Bi. The small number of such compounds suggests that a small fraction of the structural prototypes used to generate hypothetical compounds in the OQMD are well-suited to achieve a one-band correlated material. For example, Li₂ is currently the only OQMD prototype structure for which all sites of an element are in square planar coordination (e.g. the Cu site in CuAu₃). BiPd₃, Ni₃Sb, and Zr₃Bi correspond to this prototype. Mn₂TeO initially in the Pnma CaFeSeO structure relaxes to a distinct Pnma structure with linear Mn–O coordination. HfBr₃ initially in the D₀₁₉ (P6₃/mmc, Ni₃Sn-type) structure relaxes to a distinct P6₃/mmc structure with one-dimensional chains of triangular-face-sharing trigonal prismatic HfBr₆ units. CsWO₃ initially in the R₃ ilmenite (FeTiO₃-type) structure relaxes to a distinct R₃ structure with layers of edge-sharing trigonal prismatic WO₆ units arranged as a kagome lattice.

The frequency of the TM and anion elements bonded in the low-symmetry coordinations is illustrated as a network in Fig. 2(c). Here each node represents a TM or anion element and the area of the node (width of the edge) is proportional to the number of compounds containing these element(s) in the low-symmetry coordination. Copper-oxygen is the most dominant chemistry with 74 of the 187 candidate compounds. Cu and O individually are the most prevalent TM and anion, respectively, as well: Cu is the TM in 90 of the compounds and O is the anion in 101 of the compounds. However, there are still many different TMs and anions represented. The anions S, Se, N and TMs Nb, Ta, Ni, and Au each occur in at least 9 compounds. The presence of many Cu-containing and square planar compounds is consistent with a high occurrence of square planar Cu²⁺ found in a recent statistical analysis of coordination environments.

The complete list of the 187 candidate compounds is included in the Supplemental Material. We note that the presence of several known classes of correlated materials such as the cuprates (e.g. La₂CuO₄) and group-V transition metal dichalcogenides (e.g. (Nb/Ta)(S/Se)₂) is suggestive of the validity of our screening strategy.

### C. Additional screening criteria for non-cuprates with extended structures

As discussed above, a key characteristic of strongly correlated materials like the cuprates is a large $U/t$ ratio. In this regime, the Coulomb repulsion can overwhelm the electron hopping, leading to localized electronic states and Mott insulating behavior as is found in, for example, the cuprate parent compounds. In addition to a large $U/t$ ratio, a finite hopping $t$ is still necessary to ensure there is a conduction pathway. As such, we expect materials with extended crystal structures (leading to extended hopping pathways and appreciable $t$), to be necessary to achieve a one-band correlated material.

In order to search for the most promising compounds among the 187 candidates for a one-band correlated material, we therefore perform an additional post-processing screening criterion based on the crystal structures to discard any compound for which there is no connectivity (direct or indirect) between the TM–anion coordination cages. For example, K₄IrO₄ is removed since the IrO₄ square planar units are isolated, whereas TICuPO₄ is retained since the CuO₄ square planar units are connected indirectly via phosphate groups.

| Composition | Coordination |
|-------------|--------------|
| Cs WO₃      | Trig. prismatic |
| Li MoN₂     | Trig. prismatic |
| HfBr₃       | Trig. prismatic |
| Rb Fe(SeO₃)₂ | Trig. prismatic |
| K₃H (CuP₂O₇)₁₂ | Sq. pyramidal |
| Al₂F₂ CuSi₂O₇ | Sq. pyramidal |
| Ba₄(Nd/Sm)₁₀ Cu₃O₉ | Sq. pyramidal |
| Ca NiN      | Linear       |
| Sn₂ Co₃S₂   | Linear       |
| In Co₃N     | Linear       |
| (Sr/Ba) Cu(SeO₃)₁₂ | Sq. planar |
| CuBr₂       | Sq. planar   |
| (La/Gd)₁₀ Cu(SeO₃)₁₄ | Sq. planar |
| Na₂ CuP₂O₇ | Sq. planar |
| Ti Cu(P/As)O₄ | Sq. planar |
| (Sr/Pb)₂ Cu(BO₃)₁₂ | Sq. planar |
| Bi₂ Cu(SeO₃)₁₄ | Sq. planar |
| Ca₂Sb FeO₆ | Sq. planar |
| Ca(H₂O) CuSiO₄ | Sq. planar |
| Li₂ CuO₂   | Sq. planar |
| Na₃ClH CuPO₃ | Sq. planar |

**TABLE I.** The identified 26 non-cuprate candidate compounds with extended electron hopping pathways and the TM coordination environment.

Finally, we also remove materials containing any of the CuO₂ planes characteristic of the cuprates since this material class is already well studied and is not our focus. These two post-processing steps reduce the number of candidate materials from 187 to 26; these candidates are contained in Table I and also shown in the “Extended bonding” screening criterion in Fig. 1. Only trigonal prismatic, square pyramidal, linear, and square planar coordinations remain after this additional screening step and compounds with Cu bonded to O continue to dominate.
D. Electronic band structures

For each of the 26 compounds, we compute the DFT electronic band structure to assess whether the underlying one-electron electronic structure is one-band in nature. In other words, we assess which band structures contain a single half-filled $d$ band straddling the Fermi energy with separations in energy below and above the band. The non-spin-polarized band structure is computed; possible effects of magnetism and strong electronic correlations on the electronic spectra will be discussed in the following subsection.

The various screening criteria are not sufficient to ensure a one-band electronic structure, and the majority of the 26 candidates do not achieve the desired band structure. Several possible characteristics of the candidate compound can prevent the targeted band structure:

1. **Covalency:** If there is too much hybridization between the TM $d$ states and anion $p$ states, an itinerant metal is found (example: LiMoN$_2$)

2. **Metal-metal bonding:** If the crystal structure has multiple TM sites and less localized $d$ states (e.g. 5$d$), these states can hybridize and form a band insulator by completely filling a bonding orbital (example: CsWO$_3$)

3. **Distinct TM sites:** If the crystal structure has TM sites with distinct environments, one can find multiple bands instead of a single band (example: TiCuPO$_4$

The electronic spectra for these false positive cases is included in the Supplemental Material.

We find 5 materials that successfully achieve a correlated one-band electronic structure: CuBr$_2$, Li$_2$CuO$_2$, the selenate compounds BaCu(SeO$_3$)$_2$ and SrCu(SeO$_3$)$_2$, and the pyrophosphate compound K$_3$H(CuP$_2$O$_7$)$_2$. The crystal structures and corresponding band structures are depicted in Fig. 3 and the compounds correspond to the final “1-band material” screening criterion in Fig. 1. We note that there is a splitting of the half-filled band for the selenates and pyrophosphate corresponding to two slightly different TM environments, but the splitting is of very small magnitude. For example, along the high-symmetry $k$-path for SrCu(SeO$_3$)$_2$ the maximum splitting (at $\Gamma$) is only 34 meV.

All the compounds contain Cu, suggesting it is difficult to achieve a one-band correlated material with other TMs. We find that the fraction of Cu-based candidate materials in Fig. 1 increases gradually with successive filters, but the most significant increases occur for the last three (coordination, extended bonding/non-cuprate, and one-band band structure). Despite the dominance of oxygen-containing compounds, we do find one compound lacking oxygen (CuBr$_2$). We also note similarity in the local structure of the compounds: all but K$_3$H(CuP$_2$O$_7$)$_2$ have square planar coordination and K$_3$H(CuP$_2$O$_7$)$_2$ is square pyramidal, which is closely related to square planar.

The selenates and pyrophosphate are all stable or within 1 meV/atom of the ground state energy. CuBr$_2$ is highly stable: it would have to increase in energy by 230 meV/atom to become thermodynamically unstable. Li$_2$CuO$_2$ is 46 meV/atom above the ground state, but it has been experimentally synthesized. Therefore, all five of the identified compounds should be ripe for synthesis and further experimental studies.

While CuBr$_2$ is a binary compound with a simple stoichiometry, we also find compounds with much more complicated stoichiometries and structures. While CuBr$_2$ and Li$_2$CuO$_2$ have 1D chains of edge-sharing Cu–O square planar units, the selenate and pyrophosphate compounds have more complicated 2D and 3D structures. K$_3$H(CuP$_2$O$_7$)$_2$ even contains hydrogen. Our query just as easily finds these more complicated compounds, which is a strength of the informatics-driven approach to materials discovery.

E. Evidence for strong correlation physics

Finally, we discuss the possibility of strong correlation physics in the five identified materials. We note that even at the non-spin-polarized DFT level of theory, each of these 5 materials already shows potential for strong correlation physics. In particular, each has a narrow (bandwidth no more than 1.1 eV) but not completely flat (bandwidth no less than 1.1 eV) half-filled band, which is suggestive of a large $U/t$ ratio and finite $t$, of substantial $d$ orbital character. Due to the relatively large size of the primitive unit cell for (Sr/Ba)Cu(SeO$_3$)$_2$ and K$_3$H(CuP$_2$O$_7$)$_2$, a quantitative calculation of the $U$ parameter is outside the scope of this work. However, previous estimations of $U$ for copper compounds based on *ab initio* calculations and experiments suggest values will very likely be on the order of 4 eV or greater.

The non-spin-polarized band structure in Fig. 3 can be considered the underlying one-electron (band theory) electronic structure. Strong electron correlation can substantially modify the electronic structure in ways often not adequately captured by DFT, such as magnetism and Mott insulating behavior. Here we go beyond non-spin-polarized DFT and use more sophisticated calculations incorporating magnetism and explicit on-site Coulomb interaction. The goal of such calculations (which still contain significant approximations) is not to perfectly describe the electronic properties of the identified materials, but rather to determine the possibility of strong correlation physics.

In particular, we perform spin-polarized DFT+$U$ calculations on the five candidate materials. Although DFT+$U$ corresponds to a mean-field solution to the local correlation problem (exactly solved via dynamical mean-field theory) [58] it gives a baseline expectation of the overall strength of the electronic correlations at a very cheap
FIG. 3. Electronic band structure of the identified one-band correlated materials. Crystal structures and electronic band structures within DFT are shown for the five materials. For each band structure, there is a single half-filled electronic band. The band structure of BaCu(SeO₃)₂ is not shown since it appears nearly identical to that of SrCu(SeO₃)₂.

computational cost. The results of the DFT ($U=0$) and DFT+$U$ (finite $U$) calculations including spin polarization are summarized in Fig. 4, which shows the dependence of the energetics, band gap, and magnetic moment on the on-site Coulomb repulsion $U$ for the 5 candidate materials. Several aspects suggest interesting strong correlation behavior. At the spin-polarized DFT level, all but CuBr₂ exhibit a magnetic instability corresponding to the formation of local moments. All but CuBr₂ not only become magnetic, but they all fully spin polarize and open up a band gap (forming a $S=1/2$ state).

DFT+$U$ calculations for $U = 2$ and 4 eV show that for all of these materials (even the bromide), all of the different magnetic configurations (ferromagnetic and antiferromagnetic) are gapped. This suggests Mott insulating behavior in which the strong Coulomb interaction, rather than a particular magnetic configuration, leads to an insulating state. In CuBr₂ and Li₂CuO₂, antiferromagnetism is preferred over ferromagnetism as in the cuprates. In contrast, in the more complicated crystal structures (the selenates and pyrophosphate), we find that the ferromagnetic and antiferromagnetic states are essentially degenerate (less than 1 meV/atom energy different). This suggests in these materials there is a very weak magnetic coupling, as might be expected since the square planar and square pyramidal units are not in close proximity. Since the magnetic coupling goes as $t^2/U$, the weaker magnetic coupling is consistent with the smaller bandwidth for these compounds as compared to those of CuBr₂ and Li₂CuO₂.

The identified materials, whose underlying single-electron band structure is one-band in nature, exhibit a strong tendency for the formation of insulating states with fully polarized magnetic moments regardless of magnetic configuration, as well as the presence of antiferromagnetic ordering in some cases. While more accurate correlated calculations and experiments will be necessary to elucidate the true electronic structure, these results at the approximate DFT+$U$ level already represent strong evidence for the possibility of interesting strong correlation physics in these materials candidates for the rare one-band correlated material.

IV. CONCLUSIONS

We employ a materials informatics approach to search for one-band correlated materials analogous to the cuprate high-temperature superconductors. Using a query based on transition metal $d$ electron count, crystal field theory, and formation energy, we search the more than a half million real and hypothetical inorganic crystals in the Open Quantum Materials Database for synthesizable materials with an isolated half-filled $d$ band in the low-energy spectrum. Density functional theory band structure calculations illustrate that five Cu compounds, including bromide, oxide, selenate, and pyrophosphate chemistries, successfully achieve the one-
FIG. 4. Impact of electronic correlations via DFT+U on the electronic and magnetic properties of the identified materials. The relative energetics of ferromagnetic (FM) and antiferromagnetic (AFM) states, electronic band gap, and local Cu magnetic moment as a function of correlation strength U are shown for the 5 candidate materials.

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