Supplementary Material

Chemical capacitor – its concept, functionalities and limits

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1. Computational details

Computational exploration of investigated structures was done by two-step approach. Firstly, equilibrium structures were obtained. In the second step, they were used in a static (single-point) calculations of electronic density of states (DOS). All these computations were conducted at DFT level of theory with Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional[1,2] revised for solids (PBEsol)[3]. The projector-augmented-wave method[4] with appropriate pseudopotentials[5] from v.54 dataset were used as implemented in utilized by us VASP 5.4.4 code[6]. The cut-off energy of the plane wave basis set was equal to 850 eV with a self-consistent-field convergence criterion of $1 \cdot 10^{-6}$ eV. All calculation were performed for density of the k-point grid of 0.07 $Å^{-1}$ and with accurate precision. Van der Waals dispersion correction was approximately taken into consideration by DFT-D3 approach of Grimme[7]. In the case of copper compounds, their magnetic nature was taken into account by DFT+U method[8–10] (U = 5.5 eV, J = 1 eV). We have found out that rigorous application of the periodic boundary conditions for the electric field in the ***c*** crystallographic direction does not lead to very different results for the transferred charge as compared to the scenario when this condition was omitted.

At this point we would like to point out, that geometry optimization computational approach appropriate for chem-cap structures had to take into account its two-dimensionality. In the case of calculations conducted with the three-dimensional-periodic methodology, subsequent chem-cap planes had to be separated to each other with a suitably large vacuum slab. In practice, this meant that the first step was to fully optimize (ISIF=3) the equilibrium structures of used separators as a 3D solids. Then, for each chem-cap the oxidant and reductant were appropriately applied to the separator layer. Such obtained cell had two dimensions, which lengths come from calculations for the 3D separator, and the third dimension (height) which was set as large enough to ensure planes separation. Geometry optimization of all such systems were performed with fixed shape and volume of cell (ISIF=2). Such scheme was applied for most structures studied.

Calculations of the electronic DOS, phononic DOS, and critical temperatures T_c in the truncated CC setup were carried out using the Quantum ESPRESSO (QE) suite[11,12]. Perdew-Burke-Ernzerhof (PBE) optimized norm-conserving Vanderbilt (ONCV) pseudopotentials from the Pseudo Dojo library[13] were used as a basis for the density functional theory calculations. A plane-wave kinetic energy cutoff of 100 Ry for the wavefunctions and 400 Ry for the charge density and potential was used for all systems. Brillouin-zone integration involved a 18x18x1 Γ-centered k-mesh with a Methfessel-Paxston smearing width[14] of 0.02 Ry. Since our samples are 2D materials, the out-of-plane direction was sampled with only one k-point, and a vacuum slab of at least 10 Å was included. Structural optimization was considered converged when the total energy and atomic forces per atom reached tolerances of 10^{-6} Ry and 10^{-4} Ry/Å, respectively. The vacuum spacing was kept constant. Both graphene and NaCl systems were electron and hole doped until dynamic instability (i.e., the appearance of imaginary phonon modes) was reached. The dynamical matrices and linear variation of the self-consistent potential were computed using density-function perturbation theory (DFPT)[15] on the irreducible set of a regular 6x6x1 mesh. For each q-point, the electron-phonon matrix elements were calculated on a denser 54x54x1 k-mesh. The Eliashberg spectral function was calculated for a set of broadening ranging from 0 to 0.05 Ry. The superconducting critical temperature was determined using the Allen-Dynes modified McMillan formula[16], assuming a Coulomb pseudopotential of μ = 0.10 and at degauss value of 0.03. The Eliashberg spectral function (α^2F), electron-phonon coupling strength (λ), logarithmic average phonon frequency (ω_{log}), and superconducting temperature (T_c) formulas are shown below.

$$\alpha^2F(\omega) = \frac{1}{N_F}\int \frac{dkdq}{\Omega_{BZ}^2}\sum_{mnv}\left|g_{mnv}(k,q)\right|^2\delta\left(\epsilon_{nk}-\epsilon_F\right)\delta\left(\epsilon_{mk+q}-\epsilon_F\right)\delta\left(\hbar\omega-\hbar\omega_{qv}\right)$$

$$\lambda = 2\int_0^\infty \frac{\alpha^2F(\omega)}{\omega}d\omega$$

$$\omega_{\log} = \exp\left[\frac{2}{\lambda}\int_0^\infty d\omega \frac{\alpha^2F(\omega)}{\omega}\log\omega\right]$$

$$\omega_2^2 = \frac{2}{\lambda}\int \omega\alpha^2F(\omega)d\omega$$

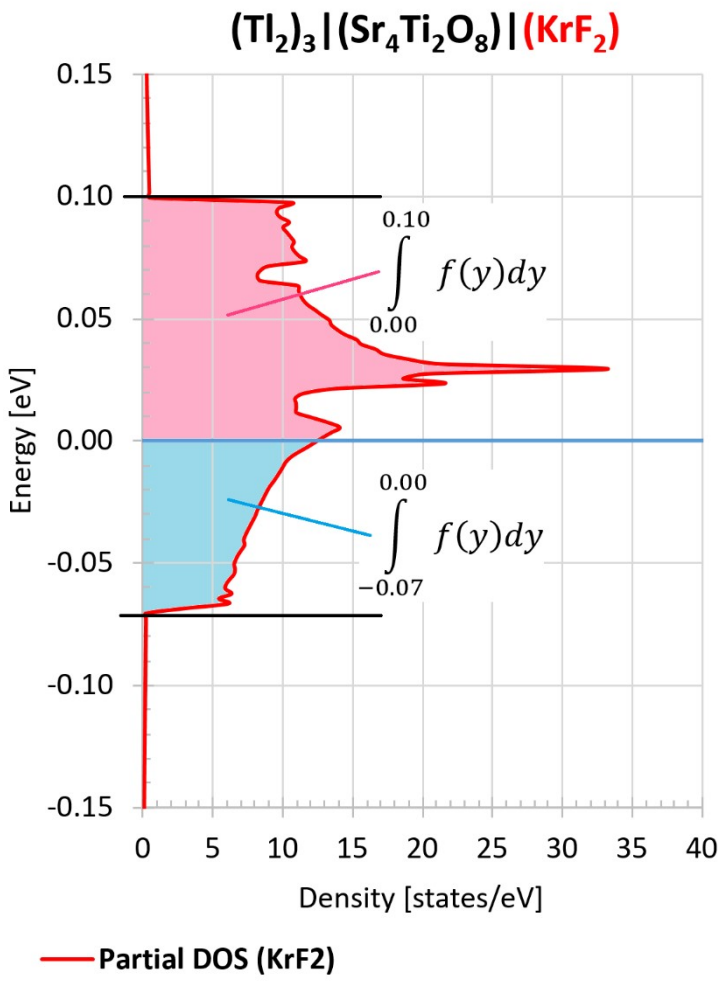
The Eliashberg spectral function ($\alpha^2F(\omega)$), the electron phonon coupling strength (λ), the logarithmic frequency (ω_{log}), and ω_2 are used to calculate the critical temperature through the modified Allen-Dynes modified McMillan formula:

$$k_B T_c = \frac{\hbar\omega_{log}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]$$

The T_C calculations for the $Mg_3Cu_7H_4$ hydride were performed using identical procedure and the same underlying physics equations but instead of employing the lambda.x code of QE they used a matdyn.x one. Brillouin-zone integration involved a 12x12x1 Γ-centered k-mesh with a smearing width of 0.01 Ry, electron – phonon matrix elements were calculated using 60x60x1 k-mesh, dynamical matrices and linear variation of the self-consistent potential were computed for 4x4x1 mesh.

All structure visualizations in this study were obtained with the VESTA software[17]. The symmetry of obtained equilibrium structures was determined with FINDSYM 7.1.3[18].

2. Charge Transfer Calculation Methodology



One of the key values determined for investigated systems is the value of charge transfer that occur in each of the studied chemical capacitors (chem-cap). Our approach to obtain its value base on partial DOS computed for the oxidizer layer (or simply for the metal center of this layer). In principle we avoid running into diverse electronic population schemes but rather we determine the charge transferred during a **redox process**, which is much simpler to calculate.

The oxidizer is as an electron acceptor. Typical result of its interaction with the reductant is filling electron shells/bands, that were empty as long as this layer was isolated from the other chem-cap parts. It is therefore crucial to examine such a partially occupied electron shell through which the Fermi level passes or are the nearest to it.

In practice, it is necessary to determine the energy limits in which this acceptor (conduction) band lies (which is only sometimes tricky) and then calculate the area of this band lying below and above the Fermi level (see Fig. above). In both cases integrals are calculated with trapezoidal rule approximation.

In the analysed example (see Fig. above), the occupied part of the band (below the Fermi level) has an area of 0.571, while the unoccupied part has an area of 1.298. In total, this gives 1.869. This band accommodates in fact exact two electrons. The deviations of obtained data are results of inaccuracy of the DOS calculation method itself. Since they mainly concern the absolute values themselves, and not their mutual relationship, the charge that found itself in this orbital can be calculated proportionally: 0.571*(2.0/1.869). This gives a final charge of 0.611 e. Since this orbital would be empty for isolated oxidizer layer, this value corresponds to the transferred charge per 1 Kr atom.

3. Brief introduction to non-stoichiometric and doped systems

Chemical matter is made up of various combinations of chemical elements, and in very different proportions. However, as Proust noted at the end of the XVIIIth century, the elements tend to combine in certain proportions that can be expressed with relatively small natural numbers[19]. The applicability of this law of definite proportions (also known as the law of constant composition), which is now more than 225 years old, ranges from the smallest systems, such as the H_2 molecule, to nanoscopic systems, such as the phosphotungstate anion $[PW_{12}O_{40}]^{3-}$ or an oligoprotein, and mezoscopic systems, such as viral RNA or other supramolecular systems, to macroscopic systems, such as a centimetre-long human chromosomal DNA molecule. To some extent, this important property of chemical matter stems from its largely molecular nature and the fact that atoms tend to form a certain small number of chemical bonds (usually with two electrons per bond). However, most non-molecular chemical systems, such as a crystal of rock salt or calcite, also follow Proust's law. Their behaviour confirms the fact that most elements tend to adopt certain integer oxidation states even in extended solids. In fact, these are mostly metals (metallic or semi-metallic elements) that bend the law slightly by forming alloys. Some, such as the coinage metals, can actually mix with each other in any ratio (Table 1). But even in the world of intermetallic compounds, there are many systems that tend to form only certain specific compositions, as is known for various Zintl-Klemm phases[20]. These can be regarded as manifestations of Pearson's principle of maximum hardness applied to solids[21].

Apart from metallic alloys, solid solutions are another exception to this law. Solid solutions are quite common among polyelement minerals, and their existence can be easily explained by the Hume-Rothery rules[22]. Namely, if two chemical elements have similar atomic sizes, crystal structures, electronegativities and valences, they easily form a solid solution either as elements or as compounds containing their ions. A classic example is lanthanide ores, which can contain all lanthanide metals in one ore. However, the formation of a solid solution does not require strict adherence to the Hume-Rothery rules. For example, the chemical composition of the mineral pyrochlore, which was found in d'Oka (Canada), can be described as follows: $(Na_{2.35}Ca_{11.01}Sr_{0.14}Mn_{0.032}Mg_{0.11}Ce_{1.36}La_{0.27}Nd_{0.34}Y_{0.016}U_{0.064}Th_{0.13}Te_{0.016})(Nb_{11.62}Ta_{0.3}Ti_{2.85}Zr_{0.24}Fe_{0.75})(O_{49.25}(OH)_{0.41}F_{6.34})$, with certainly more constituting elements occurring at much smaller concentrations. The fact that this $Ca(II)_2Nb(V)_2O_7$-type mineral adopts a highly symmetrical, "simple" space group *F*d-3m (No. 227) means that many different cations (and even those with different valences) occupy the same position in the crystal structure. In the case of the pyrochlore in question, monovalent sodium coexists at a Wyckoff position with divalent alkaline earth metals and transition metals, trivalent lanthanides, trivalent and tetravalent actinides and even with the Group 16 semimetal, tellurium"[23]. Even non-metals can form solid solutions when combined and quenched at high temperatures, as the example of $C_{1-\delta}B_\delta$ boron-doped diamond shows. The $_\delta$ in this formula can vary continuously in a certain wide range between 0 and up to about 0.25[24]. Phosphorus-doped silicon, SiP_δ, is another system in this class. In addition, phases formed by metals and ionic compounds of these metals at elevated temperature, e.g. Bi-metal and $BiCl_3$ or Cs-metal and CsI, can also be quenched[25,26]. Non-metals and their ionic salts show a similar tendency to form non-stoichiometric systems, especially for elements with large, soft atoms.

Intermetallic alloys and other solid solutions do not exhaust the list of systems that bend the law of definite proportions (Table 1). At least two other classes of systems of this type are known. One class consists of intrinsically non-stoichiometric compounds. As early as 1866, Graham recognized that hydrogen could dissolve in elemental palladium, leading to a wide range of chemical compositions, PdH_δ [27]. This is a typical feature of the so-called interstitial compounds (here H can fill certain interstices in the Pd network). $Ti_\delta O_\sigma$ and $V_\delta O_\sigma$ (here both δ and σ are non-integer values, near but not necessarily very close to unity) are other examples of non-stoichiometric systems. In fact, the formula of these phases should be written as $(M_{1-\delta}\square_\delta)(O_{1-\sigma}\square_\sigma)$ (M=Ti,V) where □ stands for a vacancy. For δ=σ, which is formally "stoichiometric", there are 16% of vacancies of both anions and cations for compounds prepared with different methods[28], *i.e.* δ=σ≈0.16. These interesting compounds owe its properties to the

thermodynamically favorable formation of vacancies at the crystallo-graphic sites of M and O driven by strong electronic correlations29.

Another family of non-stoichiometric compounds is represented by “intentionally doped” systems. These are mainly human, i.e. artificial, factories. This class is represented by the following stoichiometries, among others: $Li_\delta C$ [30], $Li_\delta MO_2$ M=Mn, Co[31], $La_{2-\delta}Ba_\delta CuO_4$ [32], $Li_\delta HfNCl$ [33], $H_\delta WO_3$ [34], $La_{1-\delta}Ca_\delta MnO_3$ [35], $Ca_{1-\delta}Y_\delta F_{2+\delta}$ [36], $(poly\text{-}C_2H_2)(I_3)_\delta$ [37] and $LaH_{10+\delta}$ [38,39]. The boundaries between these de facto informal categories are not strict, and SiP_δ can be considered as a representative of the “intentionally doped” category and at the same time as a representative of the “solid solutions of non-metals” category.

Table 1. Examples of chemical systems which break the law of definite proportions.

	Examples
Intermetallic alloys	$Cu_{0.03}Ag_{0.25}Au_{0.72}$
Quenched solid solutions of nonmetals	$C_{1-\delta}B_\delta$, SiP_δ
Quenched solid solutions of nonmetals and their salts, or metals and their salts	$Cs_{1+\delta}I$, $CsI_{1+\delta}$, $Bi_{1+\delta}Cl_\delta$
Solid solutions (compounds)	$(La_{0.15}Ce_{0.25}Pr_{0.13}Nd_{0.47})_2O_3$
Intrinsically non-stoichiometric and/or interstitial compounds	PdH_δ, $Ti_\delta O_\sigma$, $V_\delta O_\sigma$
Deliberately doped compounds	$Li_\delta C$, $Li_\delta HfNCl$, $Li_\delta MO_2$ (M=Mn, Co), $La_{2-\delta}Ba_\delta CuO_4$, $H_\delta WO_3$, $La_{1-\delta}Ca_\delta MnO_3$, $Ca_{1-\delta}Y_\delta F_{2+\delta}$, $(C_2H_2)(I_3)_\delta$, $LaH_{10+\delta}$

Properties of non-stoichiometric compounds. All the non-stoichiometric compounds mentioned above and others belonging to this family have a number of interesting physicochemical properties. One rather trivial property is density, which can vary widely across the compositional range. Occasionally, as with $Ti_\delta O_\sigma$ where $\delta=\sigma$, the density behaves quite peculiarly, being very different for TiO and $Ti_{0.9}O_{0.9}$, whereas both phases contain Ti and O in the same ratio (1:1). Another reason is the possibility of producing systems with different mechanical properties leading to different uses (just think of alloys and the copper, bronze and iron ages). However, the key feature of all non-stoichiometric materials for modern technologies is that their electrical and sometimes magnetic properties can depend dramatically on δ. Take $C_{1-\delta}B_\delta$: Boron-doped diamond is a black compound with a metallic lustre that is used as a chemically inert electrode material. On the other hand, SiP_δ or SiB_δ are usually produced with quite small δ of up to 0.01, but the precise control of δ is crucial for controlling wealth. Imagine our civilization without these n- or p-doped semiconductors and all the devices resulting from the fabrication of n-p junctions, NPJs (central processing units, CPUs, solar cells, diodes, transistors, charge-coupled devices, CCDs, in our cameras, etc.). All other materials mentioned here show the same dependence of key properties on the degree of doping. For example, $Cs_{1+\delta}I$ and $CsI_{1+\delta}$ are both metallic, while the undiluted CsI is an ionic insulator for electricity. $(La_{0.15}Ce_{0.25}Pr_{0.13}Nd_{0.47})_2O_3$ and other salts of the same type (e.g. transition metal compounds) form so-called highly entropy alloys, which exhibit a number of useful properties[40,41]. PdH_δ changes its electrical conductivity so much with δ that Pd can be used to detect traces (ppm) of H_2 gas. Other systems are no less important. $Li_\delta C$ is a member of the rich family of intercalated graphites. $Li_\delta CoO_2$ is a classic lithium storage material (first generation) for lithium batteries, $La_{2-\delta}Ba_\delta CuO_4$ is the first known high-temperature superconductor, SC, $Li_\delta HfNCl$ is also a layered SC, $H_\delta WO_3$ and $Na_\delta WO_3$ are the famous tungsten bronzes, $La_{1-\delta}Ca_\delta MnO_3$ shows huge magnetoresistance, $Ca_{1-\delta}Y_\delta F_{2+\delta}$ is an excellent fluoride ion conductor (solid electrolyte), $(poly\text{-}C_2H_2)(I_3)_\delta$ is a prototypical organic conductive polymer, while $LaH_{10+\delta}$ at a very high external pressure of 188 GPa is the first known SC with a critical temperature of 260 K (or –13 °C), approaching the melting point of ice.

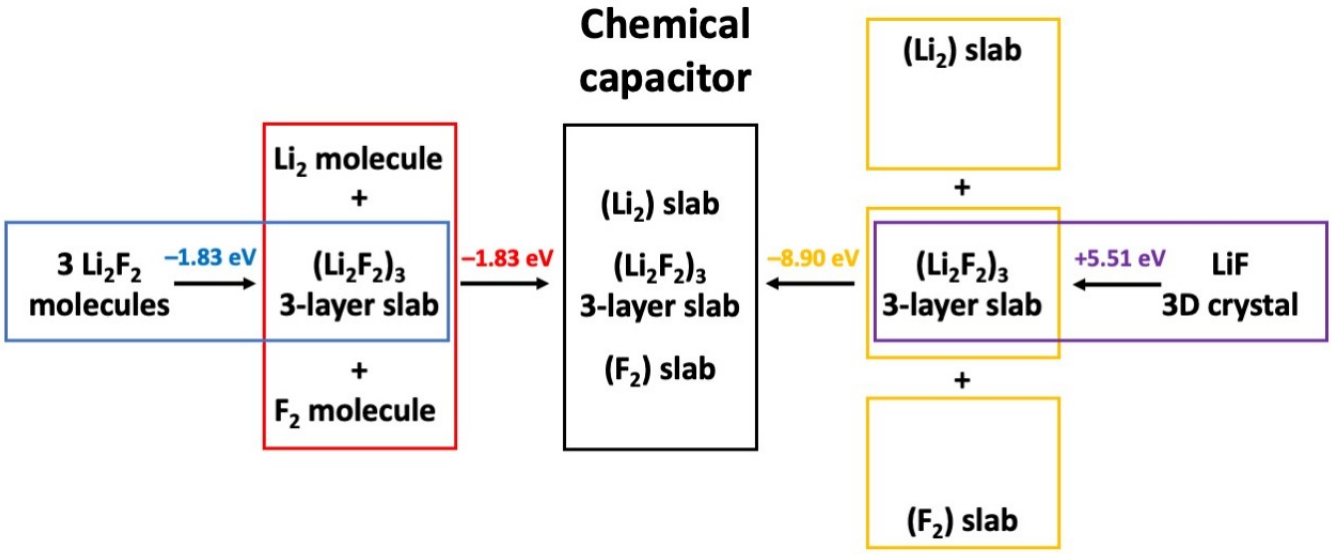
It is obvious that all non-stoichiometric systems have fascinating properties and are of immense practical importance, apart from their key role in basic research. One reason why they exhibit such peculiar properties – although they represent a minority of all chemical substances – is the fact that the formal oxidation state of at least one element in their composition is not fixed to an integer value, but depends continuously on δ. This makes $Li_\delta CoO_2$, for example, very different from Fe_3O_4, as the formal oxidation state of the transition metal changes continuously in the former, while it is fixed at 2+ and 3+ in the latter. In other words, non-stoichiometric $Li_\delta CoO_2$ represents intermediate valence (IV) systems, whereas magnetite at ambient conditions (p,T) is a classical “frozen” or mixed valence (MV) [42].

Preparation of doped materials. Non-stoichiometric doped materials can be produced using a range of physical and chemical methods. The classical approaches include: (i) co-melting, sometimes in conjunction with quenching; (ii) chemical intercalation (especially of alkali, alkaline earth and lanthanide metals) and electrochemical intercalation (especially of Li or H), (iii) introduction of defects e.g. by irradiation with vis or UV light or high-energy rays (gamma rays), (iv) reaction of material with reactive elements, e.g. H_2 (PdH_δ), H *in statu nascendi* ($H_\delta WO_3$), I_2 ($(poly\text{-}C_2H_2)(I_3)_\delta$), O_2 ($YBa_2Cu_3O_{6.5+\delta}$), F_2 ($Sr_2CuO_4F_\delta$) etc., and (v) the use of extreme pressures for the synthesis

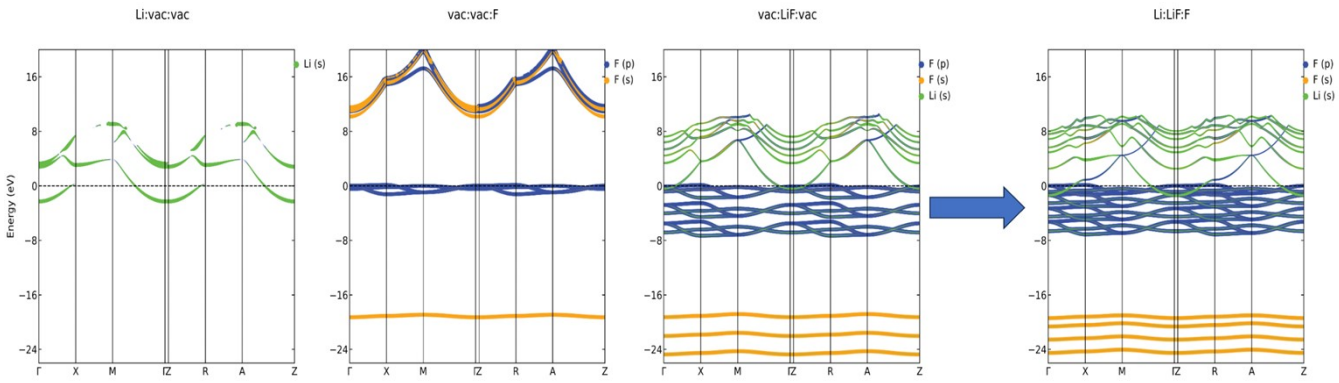
($LaH_{10+\delta}$). The use of these high-energy methods points to the difficulties that many materials have with doping, as well as their often-variable nature. Another, physical, method is to place a thin, prefabricated layer of material (sometimes only a single layer) in a strong electric field, e.g. with a field effect transistor (FET) or coming from ionic liquid transistor setup. Such devices can be used to inject electrons or holes into various substances, sometimes resulting in superconductivity[43,44,45].

4. Formation energy for the Li | $(LiF)_3$ | F system using various substrates

Note, the two entries of –1.83 eV are not a mistake but the computed values which accidentally turn out to be the same.



5. Evolution of the electronic band structure upon the formation of the Li | $(LiF)_3$ | F system



The analysis of the s and p orbital contributions using sumo package[46] from the Li, F and $(LiF)_3$ constituent layers of the Li | $(LiF)_3$ | F CC system shows in more detail what the DOS analysis (main manuscript) has already indicated. First, there are four bands for the Li layer which correspond to contribution from s orbitals of Li to $s+p^3$-based bands (strong s/p mixing scenario). Secondly, these bands are nicely split for F layer (weaker s/p mixing), where s-dominated states are found at ca. –19 eV and the three p ones at ca. –2 to 0 eV. Correspondingly, fort the isolated $(LiF)_3$ trilayer one detects three s-dominated and nine p-dominated bands, plus mostly empty states coming from Li^+ cations.

Upon the formation of the Li | $(LiF)_3$ | F CC system the number of F(s) bands increases obviously to four, and that of the F(p) states to twelve, as follows from simple summing up, but they are not a simple overlap of those for the constituent elements. Clearly, the F(p) and Li(s) orbitals from the initial F and Li layers overlap in the energy scale, which leads to the charge transfer between them, as it is also deduced from the DOS analysis.

6. CIF files of optimized structures.

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_cell_length_b     2.7954405934
_cell_length_c     30.0000000000
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_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       234.4346433375

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9 -x,-y,-z
10 -x+1/2,y,z
11 x,-y+1/2,z
12 x+1/2,y+1/2,-z
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F1  F    2 c  0.25000  0.25000  0.89961  1.00000 0,0,Dz
F2  F    2 c  0.25000  0.25000  0.03301  1.00000 0,0,Dz

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#LiF(3D)

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45 z,y,x
46 z,-y,-x
47 -z,y,-x
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114 -x+1/2,z,y+1/2
115 x+1/2,-z,y+1/2
116 x+1/2,z,-y+1/2
117 -z+1/2,-y,-x+1/2
118 -z+1/2,y,x+1/2
119 z+1/2,-y,x+1/2
120 z+1/2,y,-x+1/2
121 -x+1/2,-y,-z+1/2
122 -x+1/2,y,z+1/2
123 x+1/2,-y,z+1/2
124 x+1/2,y,-z+1/2
125 -y+1/2,-z,-x+1/2
126 -y+1/2,z,x+1/2
127 y+1/2,-z,x+1/2
128 y+1/2,z,-x+1/2
129 -z+1/2,-x,-y+1/2
130 -z+1/2,x,y+1/2
131 z+1/2,-x,y+1/2
132 z+1/2,x,-y+1/2
133 y+1/2,x,z+1/2
134 y+1/2,-x,-z+1/2
135 -y+1/2,x,-z+1/2
136 -y+1/2,-x,z+1/2
137 x+1/2,z,y+1/2
138 x+1/2,-z,-y+1/2
139 -x+1/2,z,-y+1/2
140 -x+1/2,-z,y+1/2
141 z+1/2,y,x+1/2
142 z+1/2,-y,-x+1/2
143 -z+1/2,y,-x+1/2
144 -z+1/2,-y,x+1/2
145 x+1/2,y+1/2,z
146 x+1/2,-y+1/2,-z
147 -x+1/2,y+1/2,-z
148 -x+1/2,-y+1/2,z
149 y+1/2,z+1/2,x
150 y+1/2,-z+1/2,-x
151 -y+1/2,z+1/2,-x
152 -y+1/2,-z+1/2,x
153 z+1/2,x+1/2,y
154 z+1/2,-x+1/2,-y
155 -z+1/2,x+1/2,-y
156 -z+1/2,-x+1/2,y
157 -y+1/2,-x+1/2,-z
158 -y+1/2,x+1/2,z
159 y+1/2,-x+1/2,z
160 y+1/2,x+1/2,-z
161 -x+1/2,-z+1/2,-y
162 -x+1/2,z+1/2,y
163 x+1/2,-z+1/2,y
164 x+1/2,z+1/2,-y
165 -z+1/2,-y+1/2,-x
166 -z+1/2,y+1/2,x
167 z+1/2,-y+1/2,x
168 z+1/2,y+1/2,-x
169 -x+1/2,-y+1/2,-z
170 -x+1/2,y+1/2,z
171 x+1/2,-y+1/2,z
172 x+1/2,y+1/2,-z
173 -y+1/2,-z+1/2,-x
174 -y+1/2,z+1/2,x
175 y+1/2,-z+1/2,x
176 y+1/2,z+1/2,-x
177 -z+1/2,-x+1/2,-y

```
178 -z+1/2,x+1/2,y
179 z+1/2,-x+1/2,y
180 z+1/2,x+1/2,-y
181 y+1/2,x+1/2,z
182 y+1/2,-x+1/2,-z
183 -y+1/2,x+1/2,-z
184 -y+1/2,-x+1/2,z
185 x+1/2,z+1/2,y
186 x+1/2,-z+1/2,-y
187 -x+1/2,z+1/2,-y
188 -x+1/2,-z+1/2,y
189 z+1/2,y+1/2,x
190 z+1/2,-y+1/2,-x
191 -z+1/2,y+1/2,-x
192 -z+1/2,-y+1/2,x

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li   4 b  0.50000  0.50000  0.50000  1.00000 0,0,0
F1  F    4 a  0.00000  0.00000  0.00000  1.00000 0,0,0

# end of cif
```

#Li|(LiF)$_3$|F

```
_cell_length_a     2.7954405934
_cell_length_b     2.7954405934
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       234.4346433375

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li   1 b  0.50000  0.50000  0.45947  1.00000 0,0,Dz
Li2 Li   1 a  0.00000  0.00000  0.37922  1.00000 0,0,Dz
Li3 Li   1 b  0.50000  0.50000  0.29886  1.00000 0,0,Dz
Li4 Li   1 a  0.00000  0.00000  0.21789  1.00000 0,0,Dz
F1  F    1 b  0.50000  0.50000  0.40129  1.00000 0,0,Dz
F2  F    1 a  0.00000  0.00000  0.32090  1.00000 0,0,Dz
F3  F    1 b  0.50000  0.50000  0.24045  1.00000 0,0,Dz
F4  F    1 a  0.00000  0.00000  0.15828  1.00000 0,0,Dz

# end of cif
```

#Tl|(LiF)$_3$|F

```
_cell_length_a     3.9533500000
_cell_length_b     3.9533500000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       468.8692866750

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Tl
Li
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   1 b  0.5000000000  0.5000000000  0.1478700000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.3987000000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.3186400000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.3193800000  1.0000000000 0,0,Dz
Li4 Li   2 c  0.5000000000  0.0000000000  0.2398400000  1.0000000000 0,0,Dz
F1  F    2 c  0.5000000000  0.0000000000  0.4592200000  1.0000000000 0,0,Dz
F2  F    1 b  0.5000000000  0.5000000000  0.3778500000  1.0000000000 0,0,Dz
F3  F    1 a  0.0000000000  0.0000000000  0.3783900000  1.0000000000 0,0,Dz
F4  F    2 c  0.5000000000  0.0000000000  0.2989700000  1.0000000000 0,0,Dz
F5  F    1 b  0.5000000000  0.5000000000  0.2249600000  1.0000000000 0,0,Dz
F6  F    1 a  0.0000000000  0.0000000000  0.2134700000  1.0000000000 0,0,Dz

# end of cif
```

#(Tl_4)|(Li_8F_8)$_3$|F(PtF_5)

```
_cell_length_a     7.9067000000
_cell_length_b     7.9067000000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1875.4771467000

_symmetry_space_group_name_H-M "P 1"
_symmetry_Int_Tables_number 1
_space_group.reference_setting '001:P 1'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Pt1  Pt   1 a  0.03275  0.21469  0.13832  1.00000 Dx,Dy,Dz
Li1  Li   1 a  0.01471 -0.01067  0.23482  1.00000 Dx,Dy,Dz
Li2  Li   1 a  0.00932  0.47006  0.22790  1.00000 Dx,Dy,Dz
Li3  Li   1 a  0.51220 -0.00942  0.24295  1.00000 Dx,Dy,Dz
Li4  Li   1 a  0.51081  0.48499  0.24224  1.00000 Dx,Dy,Dz
Li5  Li   1 a  0.26027  0.23470  0.23461  1.00000 Dx,Dy,Dz
Li6  Li   1 a  0.25855  0.73729  0.24278  1.00000 Dx,Dy,Dz
Li7  Li   1 a  0.77730  0.23943  0.22838  1.00000 Dx,Dy,Dz
Li8  Li   1 a  0.76491  0.73878  0.24220  1.00000 Dx,Dy,Dz
Li9  Li   1 a  0.01164  0.23805  0.31435  1.00000 Dx,Dy,Dz
Li10 Li   1 a  0.01120  0.73508  0.31017  1.00000 Dx,Dy,Dz
Li11 Li   1 a  0.51436  0.23850  0.31021  1.00000 Dx,Dy,Dz
Li12 Li   1 a  0.51257  0.73695  0.31000  1.00000 Dx,Dy,Dz
Li13 Li   1 a  0.25630 -0.00673  0.30857  1.00000 Dx,Dy,Dz
Li14 Li   1 a  0.25357  0.48149  0.30773  1.00000 Dx,Dy,Dz
Li15 Li   1 a  0.76815 -0.00420  0.30781  1.00000 Dx,Dy,Dz
Li16 Li   1 a  0.76902  0.48079  0.30818  1.00000 Dx,Dy,Dz
Li17 Li   1 a  0.01180 -0.01284  0.38360  1.00000 Dx,Dy,Dz
Li18 Li   1 a  0.01196  0.48742  0.38425  1.00000 Dx,Dy,Dz
Li19 Li   1 a  0.51244 -0.00893  0.37938  1.00000 Dx,Dy,Dz
Li20 Li   1 a  0.51177  0.48400  0.37954  1.00000 Dx,Dy,Dz
Li21 Li   1 a  0.26246  0.23787  0.38360  1.00000 Dx,Dy,Dz
Li22 Li   1 a  0.25852  0.73716  0.37939  1.00000 Dx,Dy,Dz
Li23 Li   1 a  0.76221  0.23772  0.38420  1.00000 Dx,Dy,Dz
Li24 Li   1 a  0.76565  0.73783  0.37956  1.00000 Dx,Dy,Dz
F1   F    1 a -0.01457  0.01505  0.17537  1.00000 Dx,Dy,Dz
F2   F    1 a  0.23124  0.26708  0.17534  1.00000 Dx,Dy,Dz
F3   F    1 a  0.16987  0.08011  0.10096  1.00000 Dx,Dy,Dz
F4   F    1 a  0.89174  0.35374  0.17932  1.00000 Dx,Dy,Dz
F5   F    1 a  0.83613  0.16538  0.10484  1.00000 Dx,Dy,Dz
F6   F    1 a  0.07743  0.41204  0.10471  1.00000 Dx,Dy,Dz
F7   F    1 a  0.26575 -0.01594  0.24742  1.00000 Dx,Dy,Dz
F8   F    1 a  0.26213  0.49216  0.24675  1.00000 Dx,Dy,Dz
F9   F    1 a  0.75736 -0.01242  0.24680  1.00000 Dx,Dy,Dz
F10  F    1 a  0.75678  0.49293  0.24778  1.00000 Dx,Dy,Dz
F11  F    1 a  0.01554  0.23392  0.25353  1.00000 Dx,Dy,Dz
F12  F    1 a  0.01132  0.73630  0.24715  1.00000 Dx,Dy,Dz
F13  F    1 a  0.51355  0.23823  0.24711  1.00000 Dx,Dy,Dz
F14  F    1 a  0.51141  0.73822  0.24680  1.00000 Dx,Dy,Dz
F15  F    1 a  0.26461  0.23763  0.32185  1.00000 Dx,Dy,Dz
F16  F    1 a  0.26225  0.73737  0.31787  1.00000 Dx,Dy,Dz
```

```
F17   F     1 a   0.76078   0.23777   0.32271   1.00000 Dx,Dy,Dz
F18   F     1 a   0.76145   0.73848   0.31808   1.00000 Dx,Dy,Dz
F19   F     1 a   0.01201  -0.01500   0.32185   1.00000 Dx,Dy,Dz
F20   F     1 a   0.01185   0.48881   0.32277   1.00000 Dx,Dy,Dz
F21   F     1 a   0.51222  -0.01265   0.31784   1.00000 Dx,Dy,Dz
F22   F     1 a   0.51114   0.48817   0.31805   1.00000 Dx,Dy,Dz
F23   F     1 a   0.01264   0.23695   0.39183   1.00000 Dx,Dy,Dz
F24   F     1 a   0.01216   0.73772   0.39078   1.00000 Dx,Dy,Dz
F25   F     1 a   0.51193   0.23747   0.39071   1.00000 Dx,Dy,Dz
F26   F     1 a   0.51202   0.73761   0.39038   1.00000 Dx,Dy,Dz
F27   F     1 a   0.26528  -0.01562   0.39617   1.00000 Dx,Dy,Dz
F28   F     1 a   0.26510   0.49068   0.39689   1.00000 Dx,Dy,Dz
F29   F     1 a   0.75892  -0.01545   0.39684   1.00000 Dx,Dy,Dz
F30   F     1 a   0.75884   0.49077   0.39704   1.00000 Dx,Dy,Dz
Tl1   Tl    1 a   0.30333  -0.05353   0.47689   1.00000 Dx,Dy,Dz
Tl2   Tl    1 a   0.30357   0.53225   0.47734   1.00000 Dx,Dy,Dz
Tl3   Tl    1 a   0.71756  -0.05378   0.47732   1.00000 Dx,Dy,Dz
Tl4   Tl    1 a   0.71718   0.53256   0.47741   1.00000 Dx,Dy,Dz

# end of cif
```

#$(Tl)_3|(Li_2F_2)_3|(KrF_2)$

```
_cell_length_a     3.9533500000
_cell_length_b     3.9533500000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       468.8692866750

_symmetry_space_group_name_H-M "P m m 2"
_symmetry_Int_Tables_number 25
_space_group.reference_setting '025:P 2 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z

loop_
_atom_type_symbol
Kr
Tl
Li
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Kr1 Kr   1 d  0.5000000000  0.5000000000  0.0965100000  1.0000000000 0,0,Dz
Tl1 Tl   1 c  0.5000000000  0.0000000000  0.5937900000  1.0000000000 0,0,Dz
Tl2 Tl   1 b  0.0000000000  0.5000000000  0.5313600000  1.0000000000 0,0,Dz
Tl3 Tl   1 c  0.5000000000  0.0000000000  0.4684000000  1.0000000000 0,0,Dz
Li1 Li   1 d  0.5000000000  0.5000000000  0.3718600000  1.0000000000 0,0,Dz
Li2 Li   1 a  0.0000000000  0.0000000000  0.3713200000  1.0000000000 0,0,Dz
Li3 Li   1 c  0.5000000000  0.0000000000  0.3019800000  1.0000000000 0,0,Dz
Li4 Li   1 b  0.0000000000  0.5000000000  0.3033500000  1.0000000000 0,0,Dz
Li5 Li   1 d  0.5000000000  0.5000000000  0.2288100000  1.0000000000 0,0,Dz
Li6 Li   1 a  0.0000000000  0.0000000000  0.2375700000  1.0000000000 0,0,Dz
F1  F    1 d  0.5000000000  0.5000000000  0.0310000000  1.0000000000 0,0,Dz
F2  F    1 c  0.5000000000  0.0000000000  0.3810100000  1.0000000000 0,0,Dz
F3  F    1 b  0.0000000000  0.5000000000  0.3800400000  1.0000000000 0,0,Dz
F4  F    1 c  0.5000000000  0.0000000000  0.2397800000  1.0000000000 0,0,Dz
F5  F    1 b  0.0000000000  0.5000000000  0.2404200000  1.0000000000 0,0,Dz
F6  F    1 a  0.0000000000  0.0000000000  0.3088000000  1.0000000000 0,0,Dz
F7  F    1 d  0.5000000000  0.5000000000  0.3102900000  1.0000000000 0,0,Dz
F8  F    1 d  0.5000000000  0.5000000000  0.1649300000  1.0000000000 0,0,Dz

# end of cif
```

#(Tl_2)|(Li_4F_4)$_3$|(PbO_2)$_3$

```
_cell_length_a     7.9067000000
_cell_length_b     7.9067000000
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       2500.6361956000

_symmetry_space_group_name_H-M "C m m 2"
_symmetry_Int_Tables_number 35
_space_group.reference_setting '035:C 2 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z
5 x+1/2,y+1/2,z
6 -x+1/2,-y+1/2,z
7 -x+1/2,y+1/2,z
8 x+1/2,-y+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Pb1 Pb   2 a  0.00000  0.00000  0.12693  1.00000 0,0,Dz
Pb2 Pb   2 b  0.00000  0.50000  0.15544  1.00000 0,0,Dz
Pb3 Pb   2 a  0.00000  0.00000  0.20308  1.00000 0,0,Dz
O1  O    4 e  0.00000  0.73853  0.11961  1.00000 0,Dy,Dz
O2  O    4 d  0.79725  0.00000  0.16418  1.00000 Dx,0,Dz
O3  O    4 e  0.00000  0.75321  0.21413  1.00000 0,Dy,Dz
Li1 Li   4 e  0.00000  0.73763  0.26096  1.00000 0,Dy,Dz
Li2 Li   4 e  0.00000  0.75046  0.37595  1.00000 0,Dy,Dz
Li3 Li   4 d  0.25277  0.00000  0.27381  1.00000 Dx,0,Dz
Li4 Li   2 a  0.00000  0.00000  0.31948  1.00000 0,0,Dz
Li5 Li   2 b  0.00000  0.50000  0.32093  1.00000 0,0,Dz
Li6 Li   4 c  0.25000  0.25000  0.32322  1.00000 0,0,Dz
Li7 Li   4 d  0.24931  0.00000  0.37490  1.00000 Dx,0,Dz
F1  F    4 c  0.25000  0.25000  0.27677  1.00000 0,0,Dz
F2  F    2 a  0.00000  0.00000  0.27308  1.00000 0,0,Dz
F3  F    2 b  0.00000  0.50000  0.27503  1.00000 0,0,Dz
F4  F    4 d  0.24921  0.00000  0.32809  1.00000 Dx,0,Dz
F5  F    4 e  0.00000  0.75035  0.33033  1.00000 0,Dy,Dz
F6  F    2 a  0.00000  0.00000  0.38761  1.00000 0,0,Dz
F7  F    2 b  0.00000  0.50000  0.38711  1.00000 0,0,Dz
F8  F    4 c  0.25000  0.25000  0.38154  1.00000 0,0,Dz
Tl1 Tl   2 a  0.00000  0.00000  0.44935  1.00000 0,0,Dz
Tl2 Tl   2 b  0.00000  0.50000  0.44905  1.00000 0,0,Dz

# end of cif
```

#$(Tl_4)_3|(Li_8F_8)_3|(Pb_2O_4)_5$

```
_cell_length_a     7.9067000000
_cell_length_b     7.9067000000
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       2500.6361956000

_symmetry_space_group_name_H-M "C m m 2"
_symmetry_Int_Tables_number 35
_space_group.reference_setting '035:C 2 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z
5 x+1/2,y+1/2,z
6 -x+1/2,-y+1/2,z
7 -x+1/2,y+1/2,z
8 x+1/2,-y+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Pb1 Pb   2 a  0.00000  0.00000  0.05533  1.00000 0,0,Dz
Pb2 Pb   2 b  0.00000  0.50000  0.09114  1.00000 0,0,Dz
Pb3 Pb   2 a  0.00000  0.00000  0.13178  1.00000 0,0,Dz
Pb4 Pb   2 b  0.00000  0.50000  0.17500  1.00000 0,0,Dz
Pb5 Pb   2 a  0.00000  0.00000  0.20717  1.00000 0,0,Dz
O1  O    4 e  0.00000  0.73558  0.04858  1.00000 0,Dy,Dz
O2  O    4 d  0.80577  0.00000  0.09347  1.00000 Dx,0,Dz
O3  O    4 e  0.00000  0.68308  0.13311  1.00000 0,Dy,Dz
O4  O    4 d  0.80345  0.00000  0.17127  1.00000 Dx,0,Dz
O5  O    4 e  0.00000  0.72550  0.21402  1.00000 0,Dy,Dz
Li1 Li   4 e  0.00000  0.72786  0.26173  1.00000 0,Dy,Dz
Li2 Li   4 e  0.00000  0.75040  0.37198  1.00000 0,Dy,Dz
Li3 Li   4 d  0.25674  0.00000  0.27468  1.00000 Dx,0,Dz
Li4 Li   2 a  0.00000  0.00000  0.32293  1.00000 0,0,Dz
Li5 Li   2 b  0.00000  0.50000  0.32298  1.00000 0,0,Dz
Li6 Li   4 c  0.25000  0.25000  0.32066  1.00000 0,0,Dz
Li7 Li   4 d  0.24943  0.00000  0.37172  1.00000 Dx,0,Dz
F1  F    4 c  0.25000  0.25000  0.27400  1.00000 0,0,Dz
F2  F    2 a  0.00000  0.00000  0.26696  1.00000 0,0,Dz
F3  F    2 b  0.00000  0.50000  0.27559  1.00000 0,0,Dz
F4  F    4 d  0.24684  0.00000  0.32421  1.00000 Dx,0,Dz
F5  F    4 e  0.00000  0.75243  0.32567  1.00000 0,Dy,Dz
F6  F    2 a  0.00000  0.00000  0.37655  1.00000 0,0,Dz
F7  F    2 b  0.00000  0.50000  0.37564  1.00000 0,0,Dz
F8  F    4 c  0.25000  0.25000  0.37727  1.00000 0,0,Dz
Tl1 Tl   4 c  0.25000  0.25000  0.44587  1.00000 0,0,Dz
Tl2 Tl   2 a  0.00000  0.00000  0.49221  1.00000 0,0,Dz
Tl3 Tl   2 b  0.00000  0.50000  0.49217  1.00000 0,0,Dz
Tl4 Tl   4 c  0.25000  0.25000  0.53879  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Sr_4Ti_2O_8)$|(KrF_2)

```
_cell_length_a     3.8821100000
_cell_length_b     3.8821100000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       452.1233415630

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Kr1 Kr   1 a  0.00000  0.00000  0.18796  1.00000 0,0,Dz
F1  F    1 a  0.00000  0.00000  0.26507  1.00000 0,0,Dz
F2  F    1 a  0.00000  0.00000  0.12019  1.00000 0,0,Dz
Tl1 Tl   1 b  0.50000  0.50000  0.55628  1.00000 0,0,Dz
Sr1 Sr   1 a  0.00000  0.00000  0.46563  1.00000 0,0,Dz
Sr2 Sr   1 a  0.00000  0.00000  0.33850  1.00000 0,0,Dz
Ti1 Ti   1 b  0.50000  0.50000  0.40441  1.00000 0,0,Dz
O1  O    2 c  0.50000  0.00000  0.41103  1.00000 0,0,Dz
O2  O    1 b  0.50000  0.50000  0.48134  1.00000 0,0,Dz
O3  O    1 b  0.50000  0.50000  0.34486  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Sr_4Ti_2O_8)$|(OsO_4)

```
_cell_length_a     7.7642200000
_cell_length_b     7.7642200000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1808.4933662520

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.20749  0.20749  0.57200  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51126  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.53759  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.48825  1.00000 0,0,Dz
Tl5 Tl   4 d  0.27883  0.27883  0.45665  1.00000 Dx,Dx,Dz
Sr1 Sr   2 c  0.50000  0.00000  0.37084  1.00000 0,0,Dz
Sr2 Sr   1 b  0.50000  0.50000  0.36679  1.00000 0,0,Dz
Sr3 Sr   1 a  0.00000  0.00000  0.37147  1.00000 0,0,Dz
Sr4 Sr   2 c  0.50000  0.00000  0.24878  1.00000 0,0,Dz
Sr5 Sr   1 b  0.50000  0.50000  0.21669  1.00000 0,0,Dz
Sr6 Sr   1 a  0.00000  0.00000  0.25100  1.00000 0,0,Dz
Ti1 Ti   4 d  0.25157  0.25157  0.30820  1.00000 Dx,Dx,Dz
O1  O    4 e  0.75218  0.00000  0.31459  1.00000 Dx,0,Dz
O2  O    4 f  0.75581  0.50000  0.31259  1.00000 Dx,0,Dz
O3  O    4 d  0.25494  0.25494  0.38166  1.00000 Dx,Dx,Dz
O4  O    4 d  0.24131  0.24131  0.24789  1.00000 Dx,Dx,Dz
O5  O    4 f  0.82085  0.50000  0.17507  1.00000 Dx,0,Dz
O6  O    4 e  0.31056  0.00000  0.10728  1.00000 Dx,0,Dz
Os1 Os   2 c  0.50000  0.00000  0.13720  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Sr_4Ti_2O_8)$|(RuO_4)

```
_cell_length_a     7.7642200000
_cell_length_b     7.7642200000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1808.4933662520

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.20880  0.20880  0.57265  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51162  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.53801  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.48899  1.00000 0,0,Dz
Tl5 Tl   4 d  0.27887  0.27887  0.45712  1.00000 Dx,Dx,Dz
Sr1 Sr   2 c  0.50000  0.00000  0.37050  1.00000 0,0,Dz
Sr2 Sr   1 b  0.50000  0.50000  0.36575  1.00000 0,0,Dz
Sr3 Sr   1 a  0.00000  0.00000  0.37121  1.00000 0,0,Dz
Sr4 Sr   2 c  0.50000  0.00000  0.24751  1.00000 0,0,Dz
Sr5 Sr   1 b  0.50000  0.50000  0.20095  1.00000 0,0,Dz
Sr6 Sr   1 a  0.00000  0.00000  0.24965  1.00000 0,0,Dz
Ti1 Ti   4 d  0.25120  0.25120  0.30728  1.00000 Dx,Dx,Dz
O1  O    4 e  0.75246  0.00000  0.31600  1.00000 Dx,0,Dz
O2  O    4 f  0.75729  0.50000  0.31262  1.00000 Dx,0,Dz
O3  O    4 d  0.25713  0.25713  0.38366  1.00000 Dx,Dx,Dz
O4  O    4 d  0.23502  0.23502  0.24796  1.00000 Dx,Dx,Dz
O5  O    4 f  0.82172  0.50000  0.17504  1.00000 Dx,0,Dz
O6  O    4 e  0.31217  0.00000  0.10851  1.00000 Dx,0,Dz
Ru1 Ru   2 c  0.50000  0.00000  0.13726  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Sr_4Ti_2O_8)$|(XeO_4)

```
_cell_length_a     7.7642200000
_cell_length_b     7.7642200000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1808.4933662520

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.21771  0.21771  0.57795  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51631  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.53774  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.49865  1.00000 0,0,Dz
Tl5 Tl   4 d  0.27408  0.27408  0.46172  1.00000 Dx,Dx,Dz
Sr1 Sr   2 c  0.50000  0.00000  0.37150  1.00000 0,0,Dz
Sr2 Sr   1 b  0.50000  0.50000  0.36739  1.00000 0,0,Dz
Sr3 Sr   1 a  0.00000  0.00000  0.37365  1.00000 0,0,Dz
Sr4 Sr   2 c  0.50000  0.00000  0.24088  1.00000 0,0,Dz
Sr5 Sr   1 b  0.50000  0.50000  0.19065  1.00000 0,0,Dz
Sr6 Sr   1 a  0.00000  0.00000  0.25095  1.00000 0,0,Dz
Ti1 Ti   4 d  0.25048  0.25048  0.30801  1.00000 Dx,Dx,Dz
O1  O    4 e  0.75394  0.00000  0.32031  1.00000 Dx,0,Dz
O2  O    4 f  0.75707  0.50000  0.31543  1.00000 Dx,0,Dz
O3  O    4 d  0.25884  0.25884  0.39033  1.00000 Dx,Dx,Dz
O4  O    4 d  0.22854  0.22854  0.25008  1.00000 Dx,Dx,Dz
O5  O    4 f  0.80869  0.50000  0.17440  1.00000 Dx,0,Dz
O6  O    4 e  0.30125  0.00000  0.08799  1.00000 Dx,0,Dz
Xe1 Xe   2 c  0.50000  0.00000  0.12519  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Na_4Mg_2F_8)$|(OsO_4)

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1823.0338031070

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.20222  0.20222  0.57181  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51539  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.54096  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.47936  1.00000 0,0,Dz
Tl5 Tl   4 d  0.28649  0.28649  0.45754  1.00000 Dx,Dx,Dz
Na1 Na   2 c  0.50000  0.00000  0.36867  1.00000 0,0,Dz
Na2 Na   1 b  0.50000  0.50000  0.35907  1.00000 0,0,Dz
Na3 Na   1 a  0.00000  0.00000  0.36640  1.00000 0,0,Dz
Na4 Na   2 c  0.50000  0.00000  0.25060  1.00000 0,0,Dz
Na5 Na   1 b  0.50000  0.50000  0.23928  1.00000 0,0,Dz
Na6 Na   1 a  0.00000  0.00000  0.23539  1.00000 0,0,Dz
Mg1 Mg   4 d  0.24720  0.24720  0.30974  1.00000 Dx,Dx,Dz
F1  F    4 e  0.74380  0.00000  0.32693  1.00000 Dx,0,Dz
F2  F    4 f  0.75462  0.50000  0.29926  1.00000 Dx,0,Dz
F3  F    4 d  0.29437  0.29437  0.37437  1.00000 Dx,Dx,Dz
F4  F    4 d  0.20381  0.20381  0.24829  1.00000 Dx,Dx,Dz
O1  O    4 f  0.81962  0.50000  0.17655  1.00000 Dx,0,Dz
O2  O    4 e  0.31864  0.00000  0.10973  1.00000 Dx,0,Dz
Os1 Os   2 c  0.50000  0.00000  0.14251  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Na_4Mg_2F_8)$|(RuO_4)

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1823.0338031070

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.20191  0.20191  0.57027  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51365  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.53946  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.47801  1.00000 0,0,Dz
Tl5 Tl   4 d  0.28669  0.28669  0.45604  1.00000 Dx,Dx,Dz
Na1 Na   2 c  0.50000  0.00000  0.36668  1.00000 0,0,Dz
Na2 Na   1 b  0.50000  0.50000  0.35531  1.00000 0,0,Dz
Na3 Na   1 a  0.00000  0.00000  0.36531  1.00000 0,0,Dz
Na4 Na   2 c  0.50000  0.00000  0.25001  1.00000 0,0,Dz
Na5 Na   1 b  0.50000  0.50000  0.22943  1.00000 0,0,Dz
Na6 Na   1 a  0.00000  0.00000  0.23278  1.00000 0,0,Dz
Mg1 Mg   4 d  0.24679  0.24679  0.30936  1.00000 Dx,Dx,Dz
F1  F    4 e  0.74529  0.00000  0.32725  1.00000 Dx,0,Dz
F2  F    4 f  0.75742  0.50000  0.30058  1.00000 Dx,0,Dz
F3  F    4 d  0.29455  0.29455  0.37470  1.00000 Dx,Dx,Dz
F4  F    4 d  0.20330  0.20330  0.24831  1.00000 Dx,Dx,Dz
O1  O    4 f  0.82226  0.50000  0.17961  1.00000 Dx,0,Dz
O2  O    4 e  0.32117  0.00000  0.11366  1.00000 Dx,0,Dz
Ru1 Ru   2 c  0.50000  0.00000  0.14579  1.00000 0,0,Dz

# end of cif
```

#$(Tl_2)_3$|$(Na_4Mg_2F_8)$|(XeO_4)

```
_cell_length_a     7.7642200000
_cell_length_b     7.7642200000
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1808.4933662520

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Tl1 Tl   4 d  0.20342  0.20342  0.57568  1.00000 Dx,Dx,Dz
Tl2 Tl   2 c  0.50000  0.00000  0.51688  1.00000 0,0,Dz
Tl3 Tl   1 b  0.50000  0.50000  0.54610  1.00000 0,0,Dz
Tl4 Tl   1 a  0.00000  0.00000  0.48589  1.00000 0,0,Dz
Tl5 Tl   4 d  0.28761  0.28761  0.45999  1.00000 Dx,Dx,Dz
Na1 Na   2 c  0.50000  0.00000  0.36570  1.00000 0,0,Dz
Na2 Na   1 b  0.50000  0.50000  0.35447  1.00000 0,0,Dz
Na3 Na   1 a  0.00000  0.00000  0.36980  1.00000 0,0,Dz
Na4 Na   2 c  0.50000  0.00000  0.24172  1.00000 0,0,Dz
Na5 Na   1 b  0.50000  0.50000  0.17842  1.00000 0,0,Dz
Na6 Na   1 a  0.00000  0.00000  0.23517  1.00000 0,0,Dz
Mg1 Mg   4 d  0.24524  0.24524  0.31267  1.00000 Dx,Dx,Dz
F1  F    4 e  0.75201  0.00000  0.33257  1.00000 Dx,0,Dz
F2  F    4 f  0.76484  0.50000  0.31120  1.00000 Dx,0,Dz
F3  F    4 d  0.29035  0.29035  0.38305  1.00000 Dx,Dx,Dz
F4  F    4 d  0.20287  0.20287  0.25211  1.00000 Dx,Dx,Dz
O1  O    4 f  0.81343  0.50000  0.17305  1.00000 Dx,0,Dz
O2  O    4 e  0.29079  0.00000  0.09770  1.00000 Dx,0,Dz
Xe1 Xe   2 c  0.50000  0.00000  0.13057  1.00000 0,0,Dz

# end of cif
```

 # □|($Na_8Mg_4F_{16}$)|($Cs_4Au_4Cl_{12}$)

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       2430.7117374760

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cs
Au
Cl
Na
Mg
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cs1 Cs   2 c  0.5000000000  0.0000000000  0.1193400000  1.0000000000 0,0,Dz
Cs2 Cs   2 c  0.5000000000  0.0000000000  0.2537900000  1.0000000000 0,0,Dz
Au1 Au   1 a  0.0000000000  0.0000000000  0.0549100000  1.0000000000 0,0,Dz
Au2 Au   1 b  0.5000000000  0.5000000000  0.1873500000  1.0000000000 0,0,Dz
Au3 Au   1 b  0.5000000000  0.5000000000  0.0553600000  1.0000000000 0,0,Dz
Au4 Au   1 a  0.0000000000  0.0000000000  0.3148600000  1.0000000000 0,0,Dz
Au5 Au   1 b  0.5000000000  0.5000000000  0.3246300000  1.0000000000 0,0,Dz
Au6 Au   1 a  0.0000000000  0.0000000000  0.1855800000  1.0000000000 0,0,Dz
Cl1 Cl   4 d  0.2107400000  0.2107400000  0.0565800000  1.0000000000 Dx,Dx,Dz
Cl2 Cl   4 d  0.2106800000  0.2106800000  0.3139400000  1.0000000000 Dx,Dx,Dz
Cl3 Cl   4 d  0.7107500000  0.7107500000  0.1872900000  1.0000000000 Dx,Dx,Dz
Cl4 Cl   1 b  0.5000000000  0.5000000000  0.1113700000  1.0000000000 0,0,Dz
Cl5 Cl   1 b  0.5000000000  0.5000000000  0.2689600000  1.0000000000 0,0,Dz
Cl6 Cl   1 a  0.0000000000  0.0000000000  0.2416700000  1.0000000000 0,0,Dz
Cl7 Cl   1 a  0.0000000000  0.0000000000  0.1294400000  1.0000000000 0,0,Dz
Na1 Na   4 d  0.2359000000  0.2359000000  0.3831700000  1.0000000000 Dx,Dx,Dz
Na2 Na   4 d  0.2505500000  0.2505500000  0.4718200000  1.0000000000 Dx,Dx,Dz
Mg1 Mg   1 b  0.5000000000  0.5000000000  0.4286000000  1.0000000000 0,0,Dz
Mg2 Mg   2 c  0.5000000000  0.0000000000  0.4279900000  1.0000000000 0,0,Dz
```

```
Mg3 Mg   1 a  0.0000000000  0.0000000000  0.4308700000  1.0000000000 0,0,Dz
F1  F    4 f  0.2521900000  0.5000000000  0.4271500000  1.0000000000 Dx,0,Dz
F2  F    4 e  0.2493300000  0.0000000000  0.4294600000  1.0000000000 Dx,0,Dz
F3  F    1 b  0.5000000000  0.5000000000  0.3758700000  1.0000000000 0,0,Dz
F4  F    2 c  0.5000000000  0.0000000000  0.3797500000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.3816600000  1.0000000000 0,0,Dz
F6  F    1 b  0.5000000000  0.5000000000  0.4773800000  1.0000000000 0,0,Dz
F7  F    2 c  0.5000000000  0.0000000000  0.4771000000  1.0000000000 0,0,Dz
F8  F    1 a  0.0000000000  0.0000000000  0.4793300000  1.0000000000 0,0,Dz

# end of cif
```

#(Li$_4$)|(Na$_8$Mg$_4$F$_{16}$)|(Cs$_4$Au$_4$Cl$_{12}$)

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       2430.7117374760

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cs
Au
Cl
Na
Mg
F
Li

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cs1 Cs   2 c  0.5000000000  0.0000000000  0.1173700000  1.0000000000 0,0,Dz
Cs2 Cs   2 c  0.5000000000  0.0000000000  0.2512700000  1.0000000000 0,0,Dz
Au1 Au   1 a  0.0000000000  0.0000000000  0.0538900000  1.0000000000 0,0,Dz
Au2 Au   1 b  0.5000000000  0.5000000000  0.1872900000  1.0000000000 0,0,Dz
Au3 Au   1 b  0.5000000000  0.5000000000  0.0557600000  1.0000000000 0,0,Dz
Au4 Au   1 a  0.0000000000  0.0000000000  0.3119000000  1.0000000000 0,0,Dz
Au5 Au   1 b  0.5000000000  0.5000000000  0.3245000000  1.0000000000 0,0,Dz
Au6 Au   1 a  0.0000000000  0.0000000000  0.1847500000  1.0000000000 0,0,Dz
Cl1 Cl   4 d  0.2114900000  0.2114900000  0.0554000000  1.0000000000 Dx,Dx,Dz
Cl2 Cl   4 d  0.2190100000  0.2190100000  0.3121200000  1.0000000000 Dx,Dx,Dz
Cl3 Cl   4 d  0.7109100000  0.7109100000  0.1872000000  1.0000000000 Dx,Dx,Dz
Cl4 Cl   1 b  0.5000000000  0.5000000000  0.1121100000  1.0000000000 0,0,Dz
Cl5 Cl   1 b  0.5000000000  0.5000000000  0.2684500000  1.0000000000 0,0,Dz
Cl6 Cl   1 a  0.0000000000  0.0000000000  0.2409900000  1.0000000000 0,0,Dz
Cl7 Cl   1 a  0.0000000000  0.0000000000  0.1286500000  1.0000000000 0,0,Dz
Na1 Na   4 d  0.2329000000  0.2329000000  0.3765800000  1.0000000000 Dx,Dx,Dz
Na2 Na   4 d  0.2538300000  0.2538300000  0.4693300000  1.0000000000 Dx,Dx,Dz
Mg1 Mg   1 b  0.5000000000  0.5000000000  0.4281100000  1.0000000000 0,0,Dz
```

```
Mg2 Mg   2 c  0.5000000000  0.0000000000  0.4301600000  1.0000000000 0,0,Dz
Mg3 Mg   1 a  0.0000000000  0.0000000000  0.4332000000  1.0000000000 0,0,Dz
F1  F    4 f  0.2518900000  0.5000000000  0.4326700000  1.0000000000 Dx,0,Dz
F2  F    4 e  0.2502400000  0.0000000000  0.4352100000  1.0000000000 Dx,0,Dz
F3  F    1 b  0.5000000000  0.5000000000  0.3785400000  1.0000000000 0,0,Dz
F4  F    2 c  0.5000000000  0.0000000000  0.3830000000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.3854700000  1.0000000000 0,0,Dz
F6  F    1 b  0.5000000000  0.5000000000  0.4809700000  1.0000000000 0,0,Dz
F7  F    2 c  0.5000000000  0.0000000000  0.4819400000  1.0000000000 0,0,Dz
F8  F    1 a  0.0000000000  0.0000000000  0.4837000000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.5250100000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.5242000000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.5266100000  1.0000000000 0,0,Dz

# end of cif
```

#$(Li_4)_3$|$(Na_8Mg_4F_{16})$|$(Cs_4Au_4Cl_{12})$

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     50.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       3038.3896718450

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cs
Au
Cl
Na
Mg
F
Li

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cs1 Cs   2 c  0.5000000000  0.0000000000  0.0952700000  1.0000000000 0,0,Dz
Cs2 Cs   2 c  0.5000000000  0.0000000000  0.2025000000  1.0000000000 0,0,Dz
Au1 Au   1 a  0.0000000000  0.0000000000  0.0444500000  1.0000000000 0,0,Dz
Au2 Au   1 b  0.5000000000  0.5000000000  0.1510800000  1.0000000000 0,0,Dz
Au3 Au   1 b  0.5000000000  0.5000000000  0.0456400000  1.0000000000 0,0,Dz
Au4 Au   1 a  0.0000000000  0.0000000000  0.2510400000  1.0000000000 0,0,Dz
Au5 Au   1 b  0.5000000000  0.5000000000  0.2610900000  1.0000000000 0,0,Dz
Au6 Au   1 a  0.0000000000  0.0000000000  0.1491500000  1.0000000000 0,0,Dz
Cl1 Cl   4 d  0.2113800000  0.2113800000  0.0456800000  1.0000000000 Dx,Dx,Dz
Cl2 Cl   4 d  0.2182500000  0.2182500000  0.2512100000  1.0000000000 Dx,Dx,Dz
Cl3 Cl   4 d  0.7108800000  0.7108800000  0.1510400000  1.0000000000 Dx,Dx,Dz
Cl4 Cl   1 b  0.5000000000  0.5000000000  0.0907000000  1.0000000000 0,0,Dz
Cl5 Cl   1 b  0.5000000000  0.5000000000  0.2163200000  1.0000000000 0,0,Dz
Cl6 Cl   1 a  0.0000000000  0.0000000000  0.1941500000  1.0000000000 0,0,Dz
Cl7 Cl   1 a  0.0000000000  0.0000000000  0.1042900000  1.0000000000 0,0,Dz
Na1 Na   4 d  0.2328100000  0.2328100000  0.3030600000  1.0000000000 Dx,Dx,Dz
Na2 Na   4 d  0.2535800000  0.2535800000  0.3770100000  1.0000000000 Dx,Dx,Dz
Mg1 Mg   1 b  0.5000000000  0.5000000000  0.3438400000  1.0000000000 0,0,Dz
```

```
Mg2 Mg   2 c  0.5000000000  0.0000000000  0.3452800000  1.0000000000 0,0,Dz
Mg3 Mg   1 a  0.0000000000  0.0000000000  0.3476600000  1.0000000000 0,0,Dz
F1  F    4 f  0.2518400000  0.5000000000  0.3471200000  1.0000000000 Dx,0,Dz
F2  F    4 e  0.2501500000  0.0000000000  0.3490600000  1.0000000000 Dx,0,Dz
F3  F    1 b  0.5000000000  0.5000000000  0.3040500000  1.0000000000 0,0,Dz
F4  F    2 c  0.5000000000  0.0000000000  0.3074900000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.3094100000  1.0000000000 0,0,Dz
F6  F    1 b  0.5000000000  0.5000000000  0.3855600000  1.0000000000 0,0,Dz
F7  F    2 c  0.5000000000  0.0000000000  0.3862300000  1.0000000000 0,0,Dz
F8  F    1 a  0.0000000000  0.0000000000  0.3876500000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.4209700000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.4204400000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.4222200000  1.0000000000 0,0,Dz
Li4 Li   4 d  0.2515400000  0.2515400000  0.4546800000  1.0000000000 Dx,Dx,Dz
Li5 Li   2 c  0.5000000000  0.0000000000  0.4827900000  1.0000000000 0,0,Dz
Li6 Li   1 b  0.5000000000  0.5000000000  0.4829000000  1.0000000000 0,0,Dz
Li7 Li   1 a  0.0000000000  0.0000000000  0.4832200000  1.0000000000 0,0,Dz

# end of cif
```

#($Cs_4Au_4Cl_{12}$)|($Na_8Mg_4F_{16}$)|(Xe_4F_8)

```
_cell_length_a     7.7953700000
_cell_length_b     7.7953700000
_cell_length_c     50.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       3038.3896718450

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cs
Au
Cl
Na
Mg
F
Xe

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cs1 Cs   2 c  0.5000000000  0.0000000000  0.0972800000  1.0000000000 0,0,Dz
Cs2 Cs   2 c  0.5000000000  0.0000000000  0.2050000000  1.0000000000 0,0,Dz
Au1 Au   1 a  0.0000000000  0.0000000000  0.0456600000  1.0000000000 0,0,Dz
Au2 Au   1 b  0.5000000000  0.5000000000  0.1515900000  1.0000000000 0,0,Dz
Au3 Au   1 b  0.5000000000  0.5000000000  0.0460700000  1.0000000000 0,0,Dz
Au4 Au   1 a  0.0000000000  0.0000000000  0.2534400000  1.0000000000 0,0,Dz
Au5 Au   1 b  0.5000000000  0.5000000000  0.2602600000  1.0000000000 0,0,Dz
Au6 Au   1 a  0.0000000000  0.0000000000  0.1500700000  1.0000000000 0,0,Dz
Cl1 Cl   4 d  0.2107400000  0.2107400000  0.0470500000  1.0000000000 Dx,Dx,Dz
Cl2 Cl   4 d  0.2107600000  0.2107600000  0.2525900000  1.0000000000 Dx,Dx,Dz
Cl3 Cl   4 d  0.7107200000  0.7107200000  0.1515600000  1.0000000000 Dx,Dx,Dz
Cl4 Cl   1 b  0.5000000000  0.5000000000  0.0908800000  1.0000000000 0,0,Dz
Cl5 Cl   1 b  0.5000000000  0.5000000000  0.2157600000  1.0000000000 0,0,Dz
Cl6 Cl   1 a  0.0000000000  0.0000000000  0.1948800000  1.0000000000 0,0,Dz
Cl7 Cl   1 a  0.0000000000  0.0000000000  0.1052100000  1.0000000000 0,0,Dz
Na1 Na   4 d  0.2338500000  0.2338500000  0.3080200000  1.0000000000 Dx,Dx,Dz
Na2 Na   4 d  0.2563200000  0.2563200000  0.3780200000  1.0000000000 Dx,Dx,Dz
Mg1 Mg   1 b  0.5000000000  0.5000000000  0.3425600000  1.0000000000 0,0,Dz
```

```
Mg2 Mg   2 c  0.5000000000  0.0000000000  0.3434400000  1.0000000000 0,0,Dz
Mg3 Mg   1 a  0.0000000000  0.0000000000  0.3468200000  1.0000000000 0,0,Dz
F1  F    4 f  0.2519800000  0.5000000000  0.3419700000  1.0000000000 Dx,0,Dz
F2  F    4 e  0.2491050000  0.0000000000  0.3448400000  1.0000000000 Dx,0,Dz
F3  F    1 b  0.5000000000  0.5000000000  0.3011100000  1.0000000000 0,0,Dz
F4  F    2 c  0.5000000000  0.0000000000  0.3047500000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.3069400000  1.0000000000 0,0,Dz
F6  F    1 b  0.5000000000  0.5000000000  0.3813000000  1.0000000000 0,0,Dz
F7  F    2 c  0.5000000000  0.0000000000  0.3826600000  1.0000000000 0,0,Dz
F8  F    1 a  0.0000000000  0.0000000000  0.3858100000  1.0000000000 0,0,Dz
F9  F    4 d  0.3077100000  0.3077100000  0.4223500000  1.0000000000 Dx,Dx,Dz
F10 F    4 d  0.1977000000  0.1977000000  0.5002900000  1.0000000000 Dx,Dx,Dz
Xe1 Xe   4 d  0.2497700000  0.2497700000  0.4612300000  1.0000000000 Dx,Dx,Dz

# end of cif
```

 # □|$(Li_2F_2)_3$|$(CaCuO_2)$

```
_cell_length_a     3.9533491608
_cell_length_b     3.9533491608
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       468.8690876160

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cu
O
Ca
Li
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cu1 Cu   1 a  0.0000000000  0.0000000000  0.8318900000  1.0000000000 0,0,Dz
O1  O    2 c  0.5000000000  0.0000000000  0.8374500000  1.0000000000 0,0,Dz
Ca1 Ca   1 b  0.5000000000  0.5000000000  0.8640500000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.6295900000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.6951200000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.6936800000  1.0000000000 0,0,Dz
Li4 Li   2 c  0.5000000000  0.0000000000  0.7614300000  1.0000000000 0,0,Dz
F1  F    1 b  0.5000000000  0.5000000000  0.6268100000  1.0000000000 0,0,Dz
F2  F    1 a  0.0000000000  0.0000000000  0.6268000000  1.0000000000 0,0,Dz
F3  F    2 c  0.5000000000  0.0000000000  0.6944000000  1.0000000000 0,0,Dz
F4  F    1 b  0.5000000000  0.5000000000  0.7602200000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.7600200000  1.0000000000 0,0,Dz

# end of cif
```

#(Li_2)|(Li_2F_2)$_3$|($CaCuO_2$)

```
_cell_length_a     3.9533498679
_cell_length_b     3.9533498679
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       468.8692553424

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cu
O
Ca
Li
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cu1 Cu   1 a  0.0000000000  0.0000000000  0.8425320000  1.0000000000 0,0,Dz
O1  O    2 c  0.5000000000  0.0000000000  0.8423480000  1.0000000000 0,0,Dz
Ca1 Ca   1 b  0.5000000000  0.5000000000  0.8720560000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.6256900000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.7008840000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.7000520000  1.0000000000 0,0,Dz
Li4 Li   2 c  0.5000000000  0.0000000000  0.7767910000  1.0000000000 0,0,Dz
Li5 Li   1 b  0.5000000000  0.5000000000  0.5491610000  1.0000000000 0,0,Dz
Li6 Li   1 a  0.0000000000  0.0000000000  0.5501830000  1.0000000000 0,0,Dz
F1  F    1 b  0.5000000000  0.5000000000  0.6104670000  1.0000000000 0,0,Dz
F2  F    1 a  0.0000000000  0.0000000000  0.6112510000  1.0000000000 0,0,Dz
F3  F    2 c  0.5000000000  0.0000000000  0.6862600000  1.0000000000 0,0,Dz
F4  F    1 b  0.5000000000  0.5000000000  0.7612870000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.7607290000  1.0000000000 0,0,Dz

# end of cif
```

#$(CaCuO_2)|(Li_2F_2)_3|(XeF_2)$

```
_cell_length_a     3.9533498679
_cell_length_b     3.9533498679
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       625.1590071232

_symmetry_space_group_name_H-M "P m m 2"
_symmetry_Int_Tables_number 25
_space_group.reference_setting '025:P 2 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z

loop_
_atom_type_symbol
Cu
O
Ca
Li
F
Xe

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cu1 Cu   1 a  0.0000000000  0.0000000000  0.6247670000  1.0000000000 0,0,Dz
O1  O    1 b  0.0000000000  0.5000000000  0.6293140000  1.0000000000 0,0,Dz
O2  O    1 c  0.5000000000  0.0000000000  0.6293900000  1.0000000000 0,0,Dz
Ca1 Ca   1 d  0.5000000000  0.5000000000  0.6491540000  1.0000000000 0,0,Dz
Li1 Li   1 b  0.0000000000  0.5000000000  0.4737230000  1.0000000000 0,0,Dz
Li2 Li   1 c  0.5000000000  0.0000000000  0.4722310000  1.0000000000 0,0,Dz
Li3 Li   1 d  0.5000000000  0.5000000000  0.5222320000  1.0000000000 0,0,Dz
Li4 Li   1 a  0.0000000000  0.0000000000  0.5211220000  1.0000000000 0,0,Dz
Li5 Li   1 b  0.0000000000  0.5000000000  0.5718070000  1.0000000000 0,0,Dz
Li6 Li   1 c  0.5000000000  0.0000000000  0.5715000000  1.0000000000 0,0,Dz
F1  F    1 d  0.5000000000  0.5000000000  0.4720450000  1.0000000000 0,0,Dz
F2  F    1 a  0.0000000000  0.0000000000  0.4719160000  1.0000000000 0,0,Dz
F3  F    1 b  0.0000000000  0.5000000000  0.5223450000  1.0000000000 0,0,Dz
F4  F    1 c  0.5000000000  0.0000000000  0.5221290000  1.0000000000 0,0,Dz
F5  F    1 d  0.5000000000  0.5000000000  0.5715920000  1.0000000000 0,0,Dz
F6  F    1 a  0.0000000000  0.0000000000  0.5713530000  1.0000000000 0,0,Dz
F7  F    1 c  0.5000000000  0.0000000000  0.4157290000  1.0000000000 0,0,Dz
F8  F    1 c  0.5000000000  0.0000000000  0.3133630000  1.0000000000 0,0,Dz
Xe1 Xe   1 c  0.5000000000  0.0000000000  0.3645340000  1.0000000000 0,0,Dz

# end of cif
```

#($CaCuO_2$)|(Li_2F_2)$_3$|(KrF_2)

```
_cell_length_a     3.9533498679
_cell_length_b     3.9533498679
_cell_length_c     40.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       625.1590071232

_symmetry_space_group_name_H-M "P m m 2"
_symmetry_Int_Tables_number 25
_space_group.reference_setting '025:P 2 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -x,y,z
4 x,-y,z

loop_
_atom_type_symbol
Cu
O
Ca
Li
F
Kr

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cu1 Cu   1 a  0.0000000000  0.0000000000  0.6245280000  1.0000000000 0,0,Dz
O1  O    1 b  0.0000000000  0.5000000000  0.6292430000  1.0000000000 0,0,Dz
O2  O    1 c  0.5000000000  0.0000000000  0.6292960000  1.0000000000 0,0,Dz
Ca1 Ca   1 d  0.5000000000  0.5000000000  0.6490540000  1.0000000000 0,0,Dz
Li1 Li   1 b  0.0000000000  0.5000000000  0.4729570000  1.0000000000 0,0,Dz
Li2 Li   1 c  0.5000000000  0.0000000000  0.4719200000  1.0000000000 0,0,Dz
Li3 Li   1 d  0.5000000000  0.5000000000  0.5217650000  1.0000000000 0,0,Dz
Li4 Li   1 a  0.0000000000  0.0000000000  0.5206400000  1.0000000000 0,0,Dz
Li5 Li   1 b  0.0000000000  0.5000000000  0.5712530000  1.0000000000 0,0,Dz
Li6 Li   1 c  0.5000000000  0.0000000000  0.5710940000  1.0000000000 0,0,Dz
F1  F    1 d  0.5000000000  0.5000000000  0.4717670000  1.0000000000 0,0,Dz
F2  F    1 a  0.0000000000  0.0000000000  0.4716140000  1.0000000000 0,0,Dz
F3  F    1 b  0.0000000000  0.5000000000  0.5219960000  1.0000000000 0,0,Dz
F4  F    1 c  0.5000000000  0.0000000000  0.5218800000  1.0000000000 0,0,Dz
F5  F    1 d  0.5000000000  0.5000000000  0.5713730000  1.0000000000 0,0,Dz
F6  F    1 a  0.0000000000  0.0000000000  0.5711570000  1.0000000000 0,0,Dz
F7  F    1 c  0.5000000000  0.0000000000  0.4143090000  1.0000000000 0,0,Dz
F8  F    1 c  0.5000000000  0.0000000000  0.3182110000  1.0000000000 0,0,Dz
Kr1 Kr   1 c  0.5000000000  0.0000000000  0.3661900000  1.0000000000 0,0,Dz

# end of cif
```

#$(CaCuO_2)|(Li_2F_2)_3|(F_2)$

```
_cell_length_a     3.9533498679
_cell_length_b     3.9533498679
_cell_length_c     30.0000000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       468.8692553424

_symmetry_space_group_name_H-M "P 4 m m"
_symmetry_Int_Tables_number 99
_space_group.reference_setting '099:P 4 -2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,z
4 y,-x,z
5 -x,y,z
6 x,-y,z
7 y,x,z
8 -y,-x,z

loop_
_atom_type_symbol
Cu
O
Ca
Li
F

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Cu1 Cu   1 a  0.0000000000  0.0000000000  0.8376080000  1.0000000000 0,0,Dz
O1  O    2 c  0.5000000000  0.0000000000  0.8494380000  1.0000000000 0,0,Dz
Ca1 Ca   1 b  0.5000000000  0.5000000000  0.8753210000  1.0000000000 0,0,Dz
Li1 Li   2 c  0.5000000000  0.0000000000  0.6134160000  1.0000000000 0,0,Dz
Li2 Li   1 b  0.5000000000  0.5000000000  0.6907770000  1.0000000000 0,0,Dz
Li3 Li   1 a  0.0000000000  0.0000000000  0.6887340000  1.0000000000 0,0,Dz
Li4 Li   2 c  0.5000000000  0.0000000000  0.7606890000  1.0000000000 0,0,Dz
F1  F    1 b  0.5000000000  0.5000000000  0.6277610000  1.0000000000 0,0,Dz
F2  F    1 a  0.0000000000  0.0000000000  0.6268170000  1.0000000000 0,0,Dz
F3  F    2 c  0.5000000000  0.0000000000  0.6988050000  1.0000000000 0,0,Dz
F4  F    1 b  0.5000000000  0.5000000000  0.7690960000  1.0000000000 0,0,Dz
F5  F    1 a  0.0000000000  0.0000000000  0.7696580000  1.0000000000 0,0,Dz
F6  F    2 c  0.5000000000  0.0000000000  0.5511560000  1.0000000000 0,0,Dz

# end of cif
```

#($KMgF_3$)|(NaCl)|($KMgF_3$)

```
_cell_length_a                         3.973940
_cell_length_b                         3.973940
_cell_length_c                         25.620001
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      90.000000
_cell_volume                           404.596182
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   K1         1.0     0.000000     0.000000     0.390320    Uiso  ? K
   K2         1.0     0.000000     0.000000     0.609680    Uiso  ? K
   Na1        1.0     0.500000     0.500000     0.500000    Uiso  ? Na
   Cl1        1.0     0.000000     0.000000     0.500000    Uiso  ? Cl
   F1         1.0     0.500000     0.500000     0.390320    Uiso  ? F
   F2         1.0     0.500000     0.500000     0.609680    Uiso  ? F
   F3         1.0     0.000000     0.500000     0.312531    Uiso  ? F
   F4         1.0     0.000000     0.500000     0.687469    Uiso  ? F
   F5         1.0     0.500000     0.000000     0.312531    Uiso  ? F
   F6         1.0     0.500000     0.000000     0.687469    Uiso  ? F
   Mg1        1.0     0.500000     0.500000     0.687469    Uiso  ? Mg
   Mg2        1.0     0.500000     0.500000     0.312531    Uiso  ? Mg
```

 # □| (C_2) | □

```
_cell_length_a     2.4677240000
_cell_length_b     2.4677240000
_cell_length_c     14.3425190000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  120.0000000000
_cell_volume       75.6396020518

_symmetry_space_group_name_H-M "P 6/m 2/m 2/m"
_symmetry_Int_Tables_number 191
_space_group.reference_setting '191:-P 6 2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x-y,x,z
3 -y,x-y,z
4 -x,-y,z
5 -x+y,-x,z
6 y,-x+y,z
7 x-y,-y,-z
8 x,x-y,-z
9 y,x,-z
10 -x+y,y,-z
11 -x,-x+y,-z
12 -y,-x,-z
13 -x,-y,-z
14 -x+y,-x,-z
15 y,-x+y,-z
16 x,y,-z
17 x-y,x,-z
18 -y,x-y,-z
19 -x+y,y,z
20 -x,-x+y,z
21 -y,-x,z
22 x-y,-y,z
23 x,x-y,z
24 y,x,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
C1 C   2 d  0.33333  0.66667  0.50000  1.00000 0,0,0

# end of cif
```

 # □| ($Mg_3Cu_7H_4$) | □

```
_cell_length_a     4.0100000000
_cell_length_b     4.0100000000
_cell_length_c     32.0800000000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       515.8496080000

_symmetry_space_group_name_H-M "P 4/m 2/m 2/m"
_symmetry_Int_Tables_number 123
_space_group.reference_setting '123:-P 4 2'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 -y,-x,-z
6 -y,x,z
7 y,-x,z
8 y,x,-z
9 -x,-y,-z
10 -x,y,z
11 x,-y,z
12 x,y,-z
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z

loop_
_atom_type_symbol
Mg
Cu
H

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Mg1 Mg   2 g  0.0000000000  0.0000000000  0.3750000000  1.0000000000 0,0,Dz
Mg2 Mg   1 b  0.0000000000  0.0000000000  0.5000000000  1.0000000000 0,0,0
Cu1 Cu   2 h  0.5000000000  0.5000000000  0.3750000000  1.0000000000 0,0,Dz
Cu2 Cu   4 i  0.0000000000  0.5000000000  0.4375000000  1.0000000000 0,0,Dz
Cu3 Cu   1 d  0.5000000000  0.5000000000  0.5000000000  1.0000000000 0,0,0
H1  H    2 h  0.5000000000  0.5000000000  0.4375000000  1.0000000000 0,0,Dz

# end of cif
```

7. Superconductivity parameters for NaCl layers (@ degauss 0.02).

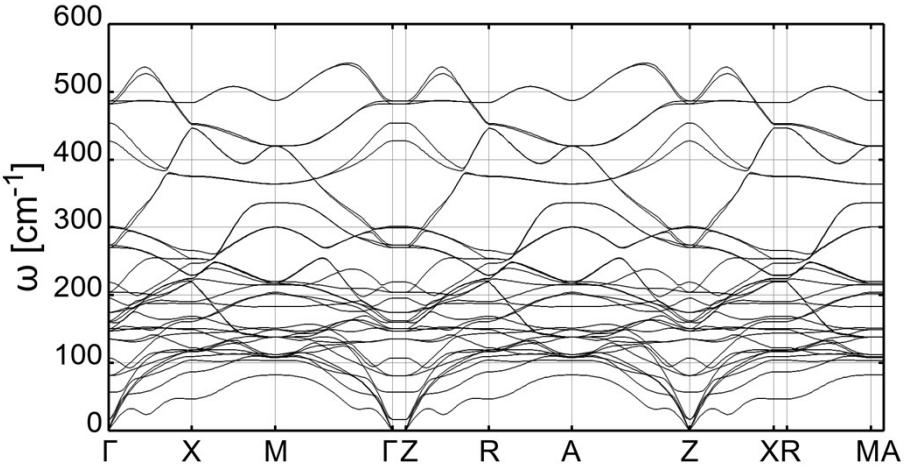
System: **($KMgF_3$) | (NaCl) | ($KMgF_3$)**	λ	N(Ef) [states/Ry]	T_C [K]
20% electron doping	0.3510	19.1898	0.216
10% hole doping	0.3138	114.8306	0.068

8. Superconductivity parameters for $Mg_3Cu_7H_4$ layers (@ degauss 0.02).

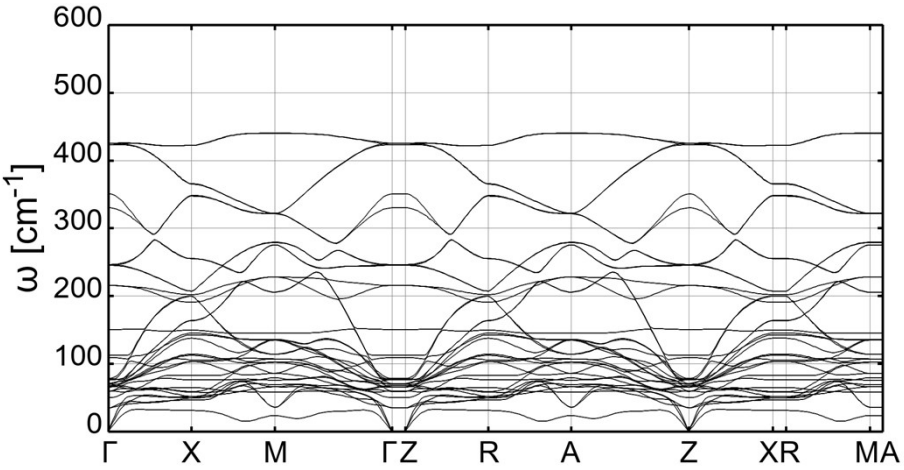
System: **□ | ($Mg_3Cu_7H_4$) | □**	λ	N(Ef) [states/Ry]	T_C [K]
10% electron doping	0.7496	14.5960	10.052
0% doping	0.7427	13.2089	11.577
10% hole doping	0.7990	12.5702	10.399

9. Phonon dispersion for NaCl layers i.e. ($KMgF_3$) | (NaCl) | ($KMgF_3$).

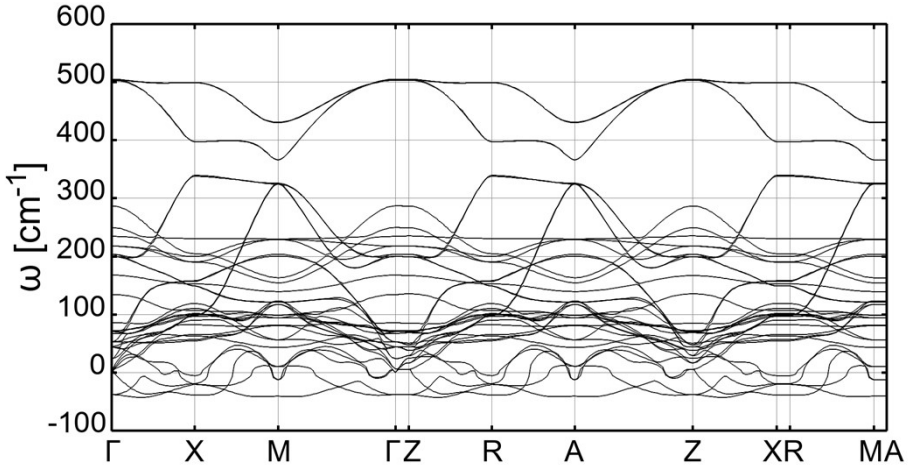
0% doping:



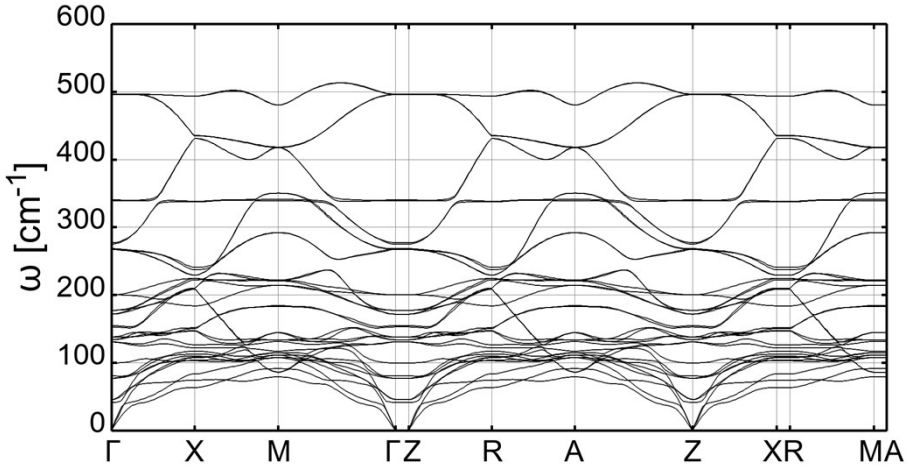
+10% doping:



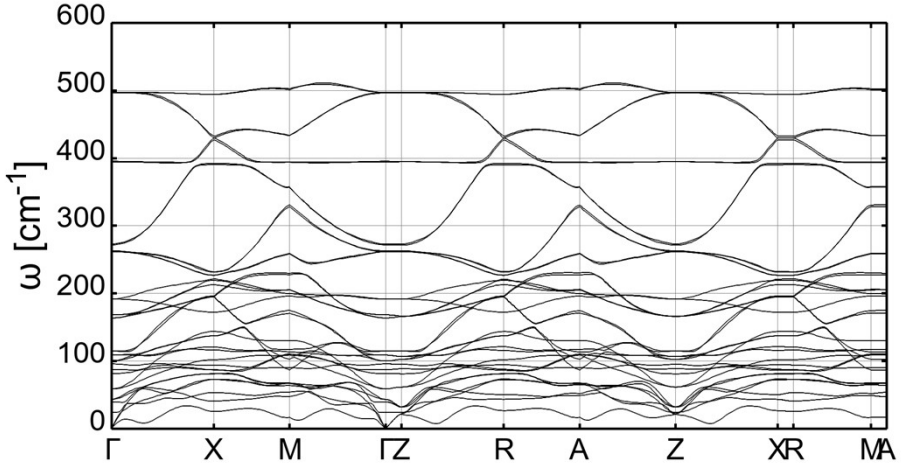
+20% doping (note the emergence of imaginary branches):



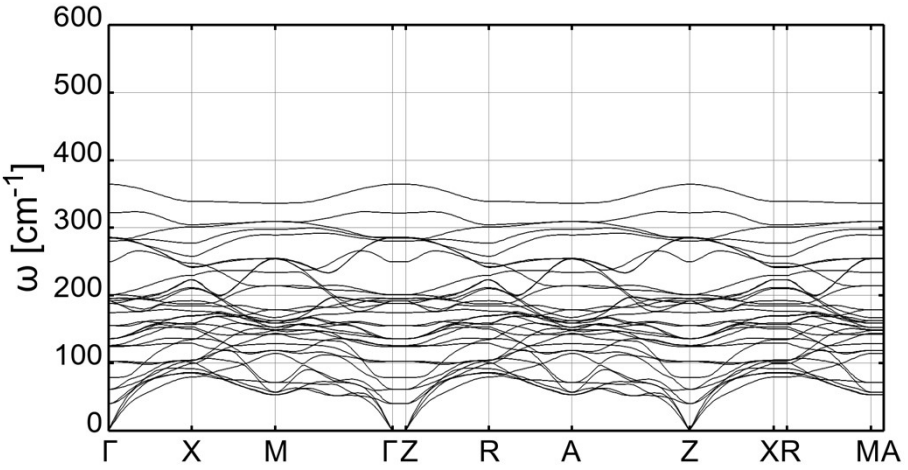
-10% doping:



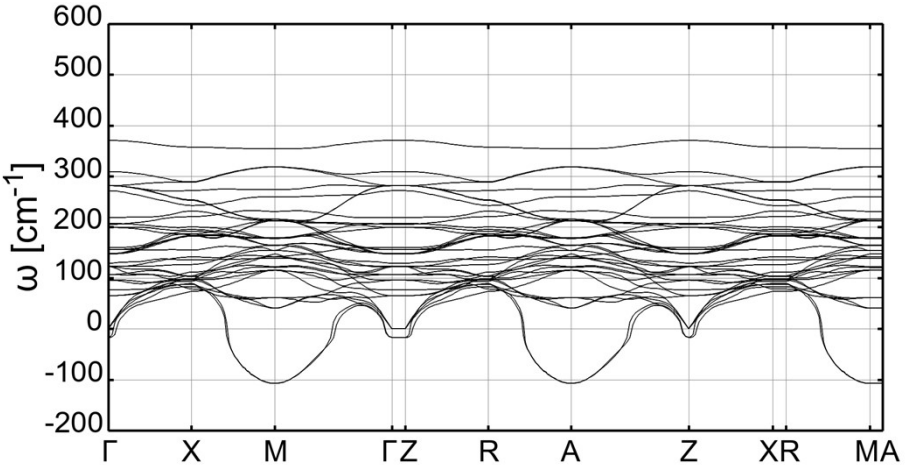
-20% doping:



-30% doping:



-40% doping (note the emergence of imaginary branches):



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