SUPPLEMENTARY INFORMATION

# Charge doping to flat $AgF_2$ monolayers in a chemical capacitor setup

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## S1. Thermodynamics of fluorination/oxidation reactions

In this section we discuss the stability of hypothetical fluorinated $AgF_2$ monolayers, in terms of the system's tendency towards decomposition into $AgF_2$ and $F_2$. We will consider only energy-preferred (GS) $AgF_{2+x}$ solutions: for RMF – flat and without distortion in the entire fluorination range; for LiF (LF) substrate – flat ($x$ = ½(I) and 1) and slightly puckered ($x$ = ¼ and ½(II)) $AgF_{2+x}$ monolayer.

The reaction (eq. 1) of fluorination of $AgF_2$ monolayer:

(Eq. 1) $AgF_2 + \frac{x}{2}F_2 \rightarrow AgF_{2+x}$

The $\Delta G$ value of fluorination reaction (eq. 1) is defined as follows:

(Eq. 2) $\Delta G_{fluor.} = G_{AgF_{2+x}} - (G_{AgF_2} + G_{\frac{x}{2}F_2})$

The enthalpy of reaction in eq. 1), calculated in the manner presented in eq. 2, enables us to estimate the stability of each $AgF_{2+x}$ monolayer, formed upon fluorination. For negative values of $\Delta G_{fluor.}$, we can expect the formation of thermodynamically stable $AgF_{2+x}$ phases. The $G_{\frac{x}{2}F_2}$ value is ground-state energy of α-$F_2$ crystal, obtained from DFT calculations, where ΔH value is equal 0.

To face experimental-related problems of fluorination, we also calculated temperature values (eq. 3), in which entropy term due to $nF_2$(gas) gas evolution is equal to energy effect (eq.2) of $AgF_2$ monolayer fluorination, considering the number of fluorine atoms involved. The standard entropy (ΔS°) for 1 mole of $F_2$ gas is equal ca. 202.8 J/mol*K.[1] It yields $\Delta G$ equal to *ca.* -1.05 meV for 0.5 molecule of $F_2$ at 1K, based on equation 3. Therefore, the temperature may be a factor by changing which, one can manipulate the degree of $AgF_2$ fluorination. Dependence of enthalpy of $AgF_2$ monolayer fluorination reaction (eq.1, eq.2) and temperatures evaluated from Eq. 3 on the degree of fluorination, are presented in the Fig. S1 (**A**) and (**B**).

(Eq. 3) $\Delta G_{\frac{x}{2}F_2} = -\frac{x}{2}TS_{(F_2 gas)}$

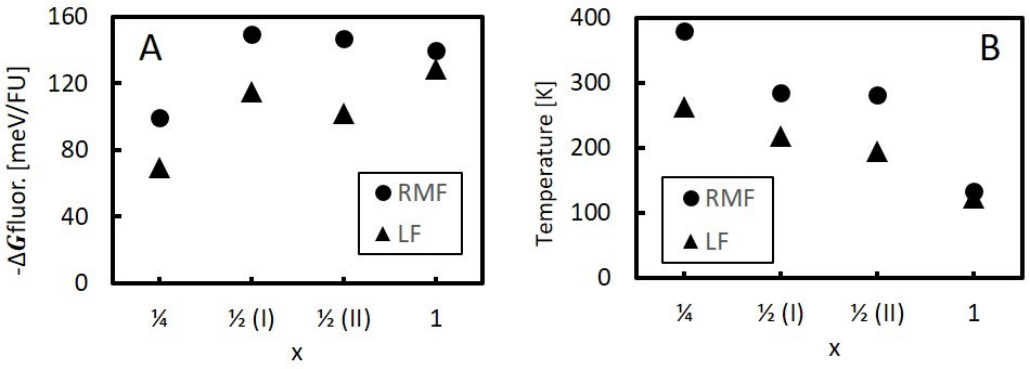


Figure S1. A – Dependence of -$^{\Delta G_{fluor.}}$ on $AgF_2$ fluorination degree (*x*) for RMF and LF substrates, B – dependence of temperature versus $AgF_2$ fluorination degree of monolayer, placed on RMF and LF.

Fig. S1 (**A**) shows the dependence of $^{\Delta G_{fluor.}}$ on degree of fluorination. The enthalpies of fluorination reactions (eq.1) are negative within the entire fluorination range studied. For LF values are slightly lower, compared to RMF. On the basis of these results, it may be tempted to state, that with Ag-Ag distance decreasing, the tendency toward fluorination increases. However, for full fluorination of $AgF_2$ monolayer, enthalpies of fluorination reaction differ only by 10.9 meV/FU between two different substrates; for RMF and LiF: ca. -139.9 meV/FU and ca. -129.0 meV/FU, respectively. This is also reflected on the values of temperatures, below which the given $AgF_{2+x}$ phase may exist. The *x* = ¼ fluorination of $AgF_2$ monolayer should be feasible around 380K and 264K for RMF and LF, respectively. As a degree of fluorination progresses, the temperature values decrease; from 218K (*x* = ½(I)) to 123K (*x* = 1), and from 285K *x* = ½(I)) to 133K (*x* = 1), for LF and RMF, respectively. Rather low values of temperatures marking stability of Ag(III) fluoride agree with the fact that $AgF_3$ prepared in the laboratory is quite thermally unstable.[ref Zemva]

In the case of indirect fluorination, the reaction is unfavorable in the entire range of *x* (fig. S2).

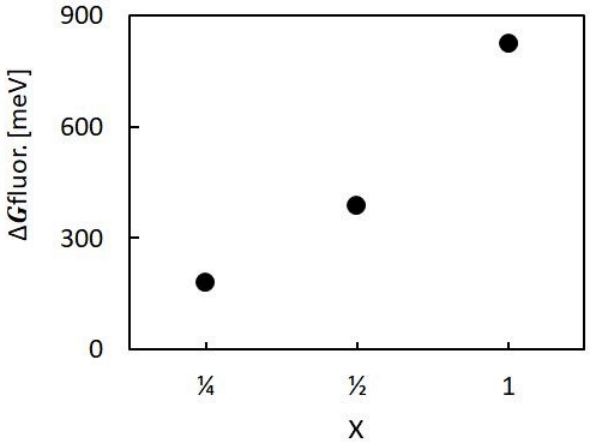


Figure S2. Dependence of $^{\Delta G_{fluor.}}$ on $AgF_2$ fluorination degree (*x*) for indirectly fluorinated LF-$AgF_2$-$Li_2F_{2+x}$ systems.

S2. Expanded eDOS graphs for hole-doped systems.

(1) Direct fluorination: RMF-$AgF_{2+x}$ and LF-$AgF_{2+x}$ systems

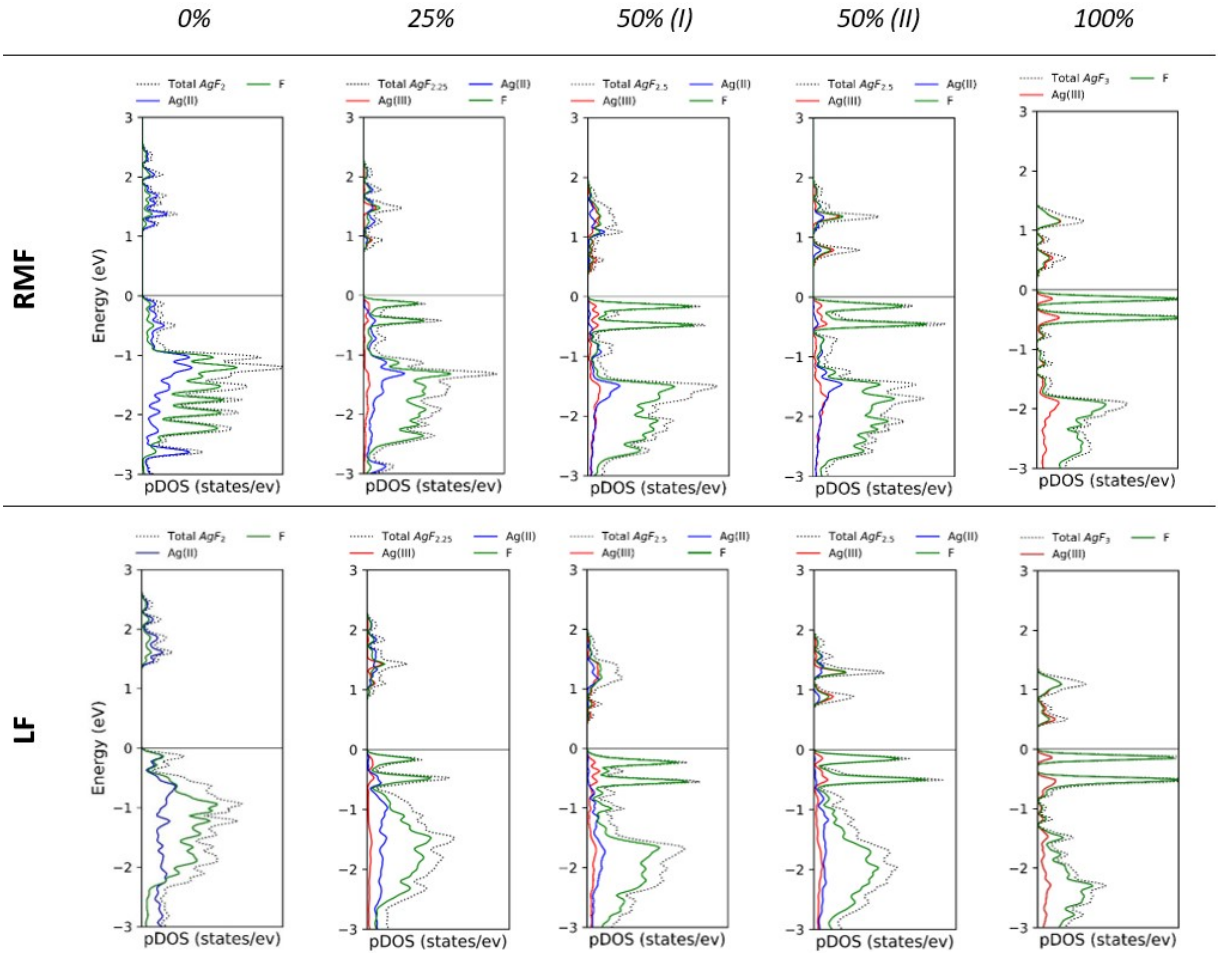


Figure S3. Atom-resolved eDOS for $AgF_{2+x}$ monolayer placed on RMF (up) and LF (down) substrate.

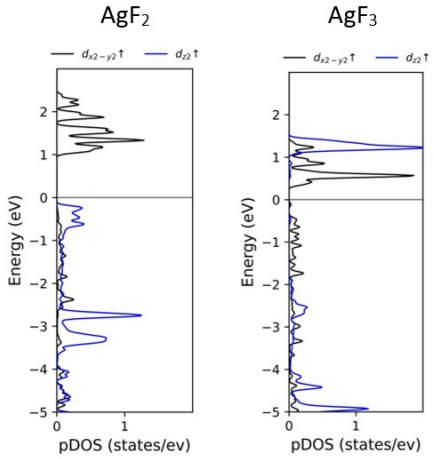


Figure S4. Orbital-resolved eDOS for $d_{x2-y2}$ and $d_{z2}$ orbitals for silver atoms from $AgF_2$ (right) and $AgF_3$ (left) monolayer placed on RMF substrate

(2) Indirect fluorination: LF-$AgF_2Li_2F_{2+x}$ systems

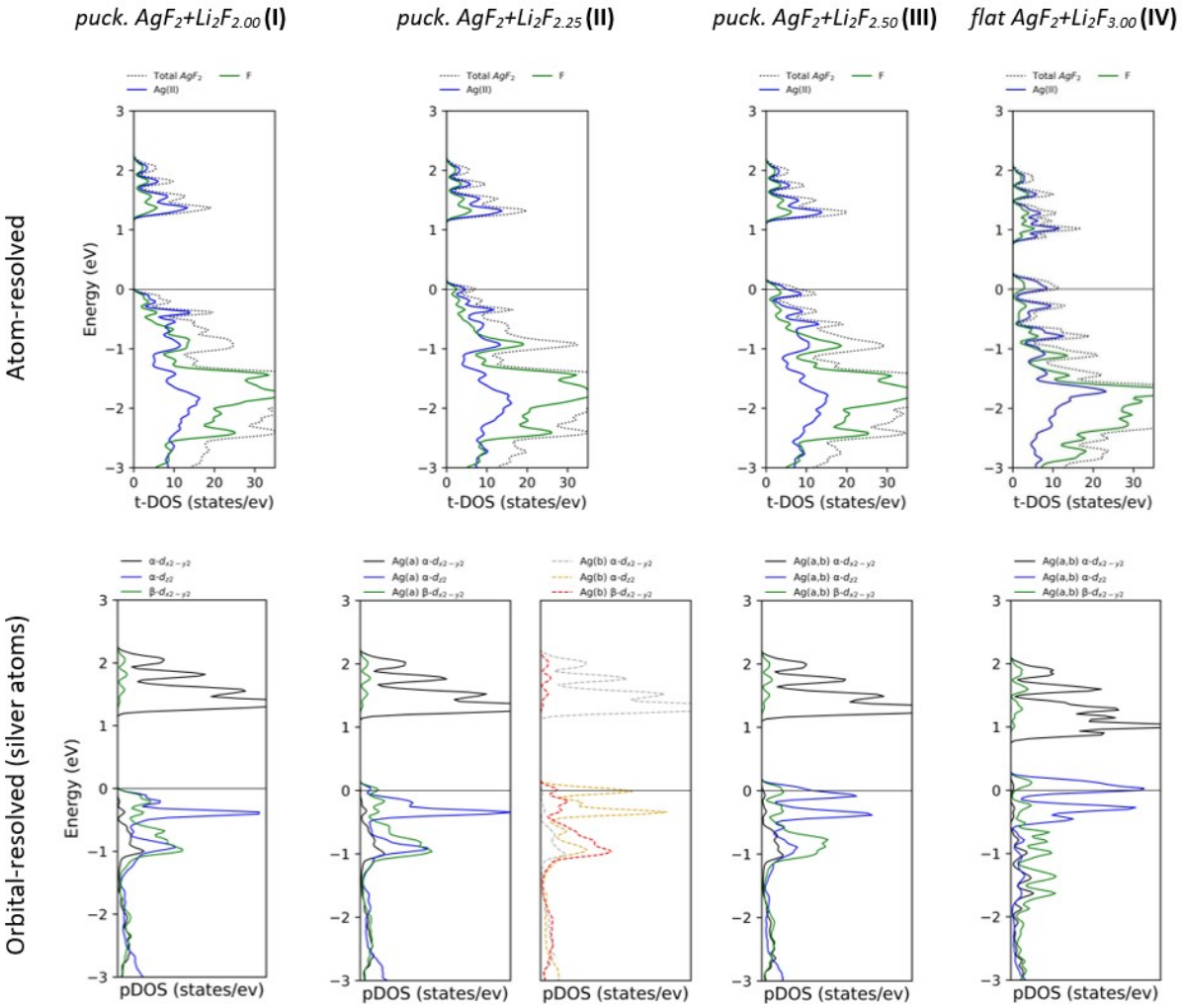


Figure S4. Atom-resolved (upper part) and orbital-resolved (lower part) eDOS for $AgF_2$ monolayer within the entire (0%, 25%, 50% and 100%) of $Li_2F_2$ atop layer fluorination.

(3) Reaction with strong oxidizer: RMF-$AgF_2$-$PtF_6$ system

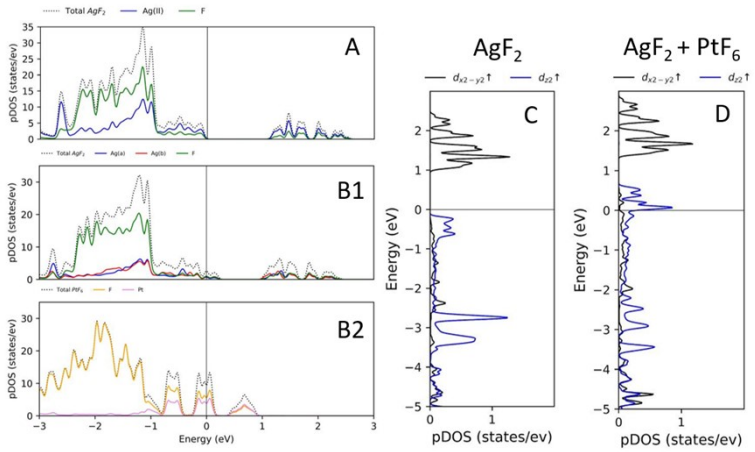


Figure S5. Atom-resolved pDOS for: (**A**) $AgF_2$ monolayer on RMF substrate, (**B1**) $AgF_2$ bonded to PtF6 molecule, and $PtF_6$ (**B2**). The right part presents orbital-resolved DOS of Ag α-$d_{x2-y2}$ and α-$d_{z2}$ states for: (**C**) pristine $AgF_2$ and (**D**) bonded to $PtF_6$ monolayer.

S3. Selected structures studied.

**$RbMgF_3$-$AgF_2$**

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Mg3 Mg 2 g 0.00000 0.00000 0.42042 1.00000 0,0,Dz
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**$RbMgF_3$-$AgF_{2.5}$ (I) ($\frac{1}{2}$ fluorination)**

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**$RbMgF_3$-$AgF_3$ (full fluorination)**

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**$RbMgF_3$-$AgF_2$-$PtF_6$ (strong oxidizer)**

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**LiF-$AgF_2$-$Li_2F_2$**

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Li8 Li 4 g 0.00000 0.66661 0.00000 1.00000 0,Dy,0
Li9 Li 4 k 0.25000 0.36102 0.25000 1.00000 0,Dy,Dz
Li10 Li 4 k 0.25000 0.36101 0.75000 1.00000 0,Dy,Dz
Li11 Li 4 g 0.00000 0.61116 0.00000 1.00000 0,Dy,0
Li12 Li 4 h 0.00000 0.38872 0.50000 1.00000 0,Dy,0
Li13 Li 4 k 0.25000 0.41673 0.75000 1.00000 0,Dy,Dz
Li14 Li 4 k 0.25000 0.58327 0.25000 1.00000 0,Dy,Dz
Li15 Li 4 g 0.00000 0.55551 0.00000 1.00000 0,Dy,0
Li16 Li 4 h 0.00000 0.55551 0.50000 1.00000 0,Dy,0
Li17 Li 4 k 0.25000 0.47224 0.75000 1.00000 0,Dy,Dz
Li18 Li 4 k 0.25000 0.52776 0.25000 1.00000 0,Dy,Dz
Li19 Li 2 b 0.00000 0.50000 0.00000 1.00000 0,0,0
Li20 Li 2 d 0.00000 0.50000 0.50000 1.00000 0,0,0
F1 F 4 k 0.25000 0.72172 0.75000 1.00000 0,Dy,Dz
F2 F 4 k 0.25000 0.27698 0.25000 1.00000 0,Dy,Dz
F3 F 4 g 0.00000 0.30570 0.00000 1.00000 0,Dy,0
F4 F 4 h 0.00000 0.69439 0.50000 1.00000 0,Dy,0
F5 F 4 k 0.25000 0.33333 0.75000 1.00000 0,Dy,Dz
F6 F 4 k 0.25000 0.66668 0.25000 1.00000 0,Dy,Dz
F7 F 4 h 0.00000 0.36104 0.50000 1.00000 0,Dy,0
F8 F 4 g 0.00000 0.63896 0.00000 1.00000 0,Dy,0
F9 F 4 k 0.25000 0.61119 0.25000 1.00000 0,Dy,Dz
F10 F 4 k 0.25000 0.61119 0.75000 1.00000 0,Dy,Dz
F11 F 4 h 0.00000 0.41673 0.50000 1.00000 0,Dy,0
F12 F 4 g 0.00000 0.41673 0.00000 1.00000 0,Dy,0
F13 F 4 k 0.25000 0.44449 0.25000 1.00000 0,Dy,Dz
F14 F 4 k 0.25000 0.55551 0.75000 1.00000 0,Dy,Dz
F15 F 4 h 0.00000 0.52776 0.50000 1.00000 0,Dy,0
F16 F 4 g 0.00000 0.47224 0.00000 1.00000 0,Dy,0
F17 F 2 f 0.25000 0.50000 0.75000 1.00000 0,0,Dz
F18 F 2 f 0.25000 0.50000 0.25000 1.00000 0,0,Dz
F19 F 4 k 0.25000 0.20700 0.25000 1.00000 0,Dy,Dz
F20 F 4 k 0.25000 0.79744 0.75000 1.00000 0,Dy,Dz
F21 F 4 g 0.00000 0.76476 0.00000 1.00000 0,Dy,0
F22 F 4 h 0.00000 0.24810 0.50000 1.00000 0,Dy,0
Ag1 Ag 4 k 0.25000 0.24168 0.25000 1.00000 0,Dy,Dz

# end of cif

**$LiF$-$AgF_2$-$Li_2F_{2.5}$ ($\frac{1}{2}$ fluorination)**

```
# CIF file created by FINDSYM, version 7.1.3

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a    5.6492174963
_cell_length_b    71.9581220000
_cell_length_c    5.6492174963
_cell_angle_alpha 90.0000000000
_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      2296.4469188569

_symmetry_space_group_name_H-M "P 1 2/m 1"
_symmetry_Int_Tables_number 10
_space_group.reference_setting '010:-P 2y'
_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_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1  Li   2 i 0.00000 0.20479 0.00000 1.00000 0,Dy,0
Li2  Li   2 l 0.50000 0.20296 0.50000 1.00000 0,Dy,0
Li3  Li   2 k 0.00000 0.20651 0.50000 1.00000 0,Dy,0
Li4  Li   2 j 0.50000 0.20234 0.00000 1.00000 0,Dy,0
Li5  Li   2 i 0.00000 0.27890 0.00000 1.00000 0,Dy,0
Li6  Li   2 l 0.50000 0.27665 0.50000 1.00000 0,Dy,0
Li7  Li   2 k 0.00000 0.27903 0.50000 1.00000 0,Dy,0
Li8  Li   2 j 0.50000 0.27693 0.00000 1.00000 0,Dy,0
Li9  Li   4 o 0.25000 0.30577 0.25000 1.00000 Dx,Dy,Dz
```

Li10 Li 4 o 0.75000 0.30529 0.25000 1.00000 Dx,Dy,Dz
Li11 Li 2 l 0.50000 0.33325 0.50000 1.00000 0,Dy,0
Li12 Li 2 i 0.00000 0.33349 0.00000 1.00000 0,Dy,0
Li13 Li 2 k 0.00000 0.33336 0.50000 1.00000 0,Dy,0
Li14 Li 2 j 0.50000 0.33330 0.00000 1.00000 0,Dy,0
Li15 Li 4 o 0.75000 0.36101 0.75000 1.00000 Dx,Dy,Dz
Li16 Li 4 o 0.25000 0.36098 0.75000 1.00000 Dx,Dy,Dz
Li17 Li 2 i 0.00000 0.38881 0.00000 1.00000 0,Dy,0
Li18 Li 2 l 0.50000 0.38881 0.50000 1.00000 0,Dy,0
Li19 Li 2 k 0.00000 0.38886 0.50000 1.00000 0,Dy,0
Li20 Li 2 j 0.50000 0.38863 0.00000 1.00000 0,Dy,0
Li21 Li 4 o 0.25000 0.41673 0.75000 1.00000 Dx,Dy,Dz
Li22 Li 4 o 0.25000 0.41673 0.25000 1.00000 Dx,Dy,Dz
Li23 Li 2 i 0.00000 0.44449 0.00000 1.00000 0,Dy,0
Li24 Li 2 j 0.50000 0.44449 0.00000 1.00000 0,Dy,0
Li25 Li 2 l 0.50000 0.44449 0.50000 1.00000 0,Dy,0
Li26 Li 2 k 0.00000 0.44449 0.50000 1.00000 0,Dy,0
Li27 Li 4 o 0.25000 0.47224 0.75000 1.00000 Dx,Dy,Dz
Li28 Li 4 o 0.25000 0.47224 0.25000 1.00000 Dx,Dy,Dz
Li29 Li 1 b 0.00000 0.50000 0.00000 1.00000 0,0,0
Li30 Li 1 e 0.50000 0.50000 0.00000 1.00000 0,0,0
Li31 Li 1 h 0.50000 0.50000 0.50000 1.00000 0,0,0
Li32 Li 1 f 0.00000 0.50000 0.50000 1.00000 0,0,0
F1 F 4 o 0.75000 0.27831 0.25000 1.00000 Dx,Dy,Dz
F2 F 4 o 0.75000 0.27661 0.75000 1.00000 Dx,Dy,Dz
F3 F 2 k 0.00000 0.30563 0.50000 1.00000 0,Dy,0
F4 F 2 i 0.00000 0.30570 0.00000 1.00000 0,Dy,0
F5 F 2 j 0.50000 0.30551 0.00000 1.00000 0,Dy,0
F6 F 2 l 0.50000 0.30559 0.50000 1.00000 0,Dy,0
F7 F 4 o 0.25000 0.33331 0.75000 1.00000 Dx,Dy,Dz
F8 F 4 o 0.25000 0.33332 0.25000 1.00000 Dx,Dy,Dz
F9 F 2 l 0.50000 0.36097 0.50000 1.00000 0,Dy,0
F10 F 2 j 0.50000 0.36104 0.00000 1.00000 0,Dy,0
F11 F 2 i 0.00000 0.36097 0.00000 1.00000 0,Dy,0
F12 F 2 k 0.00000 0.36105 0.50000 1.00000 0,Dy,0
F13 F 4 o 0.25000 0.38881 0.25000 1.00000 Dx,Dy,Dz
F14 F 4 o 0.75000 0.38880 0.25000 1.00000 Dx,Dy,Dz
F15 F 2 l 0.50000 0.41673 0.50000 1.00000 0,Dy,0
F16 F 2 k 0.00000 0.41673 0.50000 1.00000 0,Dy,0
F17 F 2 j 0.50000 0.41673 0.00000 1.00000 0,Dy,0
F18 F 2 i 0.00000 0.41673 0.00000 1.00000 0,Dy,0
F19 F 4 o 0.75000 0.44449 0.75000 1.00000 Dx,Dy,Dz
F20 F 4 o 0.75000 0.44449 0.25000 1.00000 Dx,Dy,Dz
F21 F 2 j 0.50000 0.47224 0.00000 1.00000 0,Dy,0
F22 F 2 k 0.00000 0.47224 0.50000 1.00000 0,Dy,0
F23 F 2 l 0.50000 0.47224 0.50000 1.00000 0,Dy,0
F24 F 2 i 0.00000 0.47224 0.00000 1.00000 0,Dy,0
F25 F 2 n 0.75000 0.50000 0.25000 1.00000 Dx,0,Dz

F26  F    2 n 0.25000 0.50000 0.25000 1.00000 Dx,0,Dz
F27  F    4 o 0.73475 0.20839 0.74501 1.00000 Dx,Dy,Dz
F28  F    4 o 0.74444 0.20328 0.25411 1.00000 Dx,Dy,Dz
F29  F    2 i 0.00000 0.82060 0.00000 1.00000 0,Dy,0
F30  F    2 i 0.00000 0.23564 0.00000 1.00000 0,Dy,0
F31  F    2 k 0.00000 0.23544 0.50000 1.00000 0,Dy,0
F32  F    2 l 0.50000 0.24813 0.50000 1.00000 0,Dy,0
F33  F    2 j 0.50000 0.24809 0.00000 1.00000 0,Dy,0
Ag1  Ag   4 o 0.25000 0.75855 0.25000 1.00000 Dx,Dy,Dz

# end of cif

**LiF-$AgF_2$-$Li_2F_3$ (full fluorination)**

# CIF file created by FINDSYM, version 7.1.3

data_findsym-output
_audit_creation_method FINDSYM

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_cell_length_b    71.9581220000
_cell_length_c    5.6492200000
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_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      2296.4489544370

_symmetry_space_group_name_H-M "P 1 2/m 1"
_symmetry_Int_Tables_number 10
_space_group.reference_setting '010:-P 2y'
_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_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

```
_atom_site_occupancy
_atom_site_fract_symmform
Li1  Li   2 k 0.00000 0.20634 0.50000 1.00000 0,Dy,0
Li2  Li   2 j 0.50000 0.20328 0.00000 1.00000 0,Dy,0
Li3  Li   2 i 0.00000 0.20511 0.00000 1.00000 0,Dy,0
Li4  Li   2 l 0.50000 0.20023 0.50000 1.00000 0,Dy,0
Li5  Li   2 k 0.00000 0.27874 0.50000 1.00000 0,Dy,0
Li6  Li   2 j 0.50000 0.27648 0.00000 1.00000 0,Dy,0
Li7  Li   2 i 0.00000 0.27854 0.00000 1.00000 0,Dy,0
Li8  Li   2 l 0.50000 0.27642 0.50000 1.00000 0,Dy,0
Li9  Li   4 o 0.25000 0.30575 0.75000 1.00000 Dx,Dy,Dz
Li10 Li   4 o 0.75000 0.30522 0.75000 1.00000 Dx,Dy,Dz
Li11 Li   2 j 0.50000 0.33323 0.00000 1.00000 0,Dy,0
Li12 Li   2 k 0.00000 0.33339 0.50000 1.00000 0,Dy,0
Li13 Li   2 i 0.00000 0.33333 0.00000 1.00000 0,Dy,0
Li14 Li   2 l 0.50000 0.33328 0.50000 1.00000 0,Dy,0
Li15 Li   4 o 0.75000 0.36099 0.25000 1.00000 Dx,Dy,Dz
Li16 Li   4 o 0.25000 0.36095 0.25000 1.00000 Dx,Dy,Dz
Li17 Li   2 k 0.00000 0.38881 0.50000 1.00000 0,Dy,0
Li18 Li   2 j 0.50000 0.38880 0.00000 1.00000 0,Dy,0
Li19 Li   2 i 0.00000 0.38886 0.00000 1.00000 0,Dy,0
Li20 Li   2 l 0.50000 0.38863 0.50000 1.00000 0,Dy,0
Li21 Li   4 o 0.25000 0.41673 0.25000 1.00000 Dx,Dy,Dz
Li22 Li   4 o 0.25000 0.41673 0.75000 1.00000 Dx,Dy,Dz
Li23 Li   2 k 0.00000 0.44449 0.50000 1.00000 0,Dy,0
Li24 Li   2 l 0.50000 0.44449 0.50000 1.00000 0,Dy,0
Li25 Li   2 j 0.50000 0.44449 0.00000 1.00000 0,Dy,0
Li26 Li   2 i 0.00000 0.44449 0.00000 1.00000 0,Dy,0
Li27 Li   4 o 0.25000 0.47224 0.25000 1.00000 Dx,Dy,Dz
Li28 Li   4 o 0.25000 0.47224 0.75000 1.00000 Dx,Dy,Dz
Li29 Li   1 f 0.00000 0.50000 0.50000 1.00000 0,0,0
Li30 Li   1 h 0.50000 0.50000 0.50000 1.00000 0,0,0
Li31 Li   1 e 0.50000 0.50000 0.00000 1.00000 0,0,0
Li32 Li   1 b 0.00000 0.50000 0.00000 1.00000 0,0,0
F1   F    4 o 0.75000 0.27828 0.75000 1.00000 Dx,Dy,Dz
F2   F    4 o 0.75000 0.27630 0.25000 1.00000 Dx,Dy,Dz
F3   F    2 i 0.00000 0.30551 0.00000 1.00000 0,Dy,0
F4   F    2 k 0.00000 0.30562 0.50000 1.00000 0,Dy,0
F5   F    2 l 0.50000 0.30529 0.50000 1.00000 0,Dy,0
F6   F    2 j 0.50000 0.30553 0.00000 1.00000 0,Dy,0
F7   F    4 o 0.25000 0.33330 0.25000 1.00000 Dx,Dy,Dz
F8   F    4 o 0.25000 0.33328 0.75000 1.00000 Dx,Dy,Dz
F9   F    2 j 0.50000 0.36094 0.00000 1.00000 0,Dy,0
F10  F    2 l 0.50000 0.36103 0.50000 1.00000 0,Dy,0
F11  F    2 k 0.00000 0.36095 0.50000 1.00000 0,Dy,0
F12  F    2 i 0.00000 0.36104 0.00000 1.00000 0,Dy,0
F13  F    4 o 0.25000 0.38880 0.75000 1.00000 Dx,Dy,Dz
F14  F    4 o 0.75000 0.38880 0.75000 1.00000 Dx,Dy,Dz
```

F15 F 2 j 0.50000 0.41673 0.00000 1.00000 0,Dy,0
F16 F 2 i 0.00000 0.41673 0.00000 1.00000 0,Dy,0
F17 F 2 l 0.50000 0.41673 0.50000 1.00000 0,Dy,0
F18 F 2 k 0.00000 0.41673 0.50000 1.00000 0,Dy,0
F19 F 4 o 0.75000 0.44449 0.25000 1.00000 Dx,Dy,Dz
F20 F 4 o 0.75000 0.44449 0.75000 1.00000 Dx,Dy,Dz
F21 F 2 l 0.50000 0.47224 0.50000 1.00000 0,Dy,0
F22 F 2 i 0.00000 0.47224 0.00000 1.00000 0,Dy,0
F23 F 2 j 0.50000 0.47224 0.00000 1.00000 0,Dy,0
F24 F 2 k 0.00000 0.47224 0.50000 1.00000 0,Dy,0
F25 F 2 n 0.75000 0.50000 0.75000 1.00000 Dx,0,Dz
F26 F 2 n 0.25000 0.50000 0.75000 1.00000 Dx,0,Dz
F27 F 4 o 0.73549 0.20975 0.24959 1.00000 Dx,Dy,Dz
F28 F 4 o 0.75166 0.20534 0.74964 1.00000 Dx,Dy,Dz
F29 F 2 k 0.00000 0.81897 0.50000 1.00000 0,Dy,0
F30 F 2 j 0.50000 0.82161 0.00000 1.00000 0,Dy,0
F31 F 2 k 0.00000 0.23715 0.50000 1.00000 0,Dy,0
F32 F 2 i 0.00000 0.23687 0.00000 1.00000 0,Dy,0
F33 F 2 j 0.50000 0.24806 0.00000 1.00000 0,Dy,0
F34 F 2 l 0.50000 0.24828 0.50000 1.00000 0,Dy,0
Ag1 Ag 4 o 0.25000 0.75830 0.75000 1.00000 Dx,Dy,Dz

# end of cif

References:

1 M. W. Chase, *NIST-JANAF Thermochemical Tables, Fourth Edition*, National Institute of Standards and Technology, Gaithersburg, MD, U.S.A, 1998.