

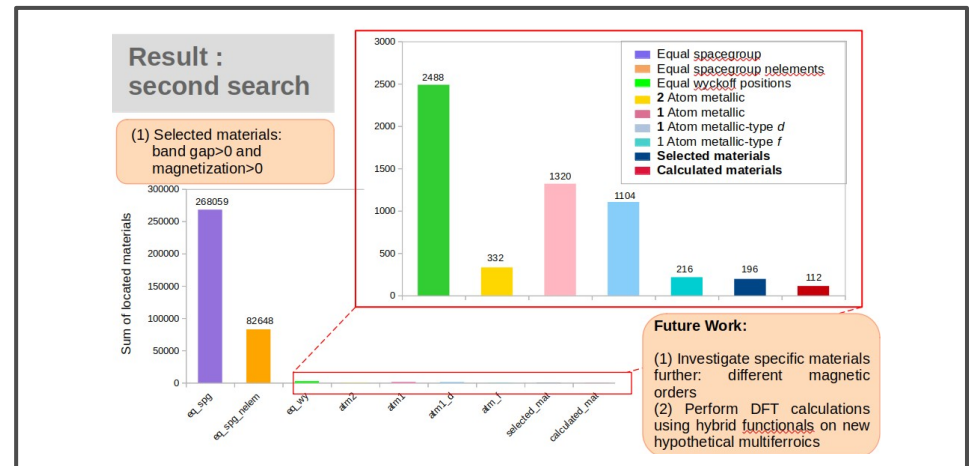
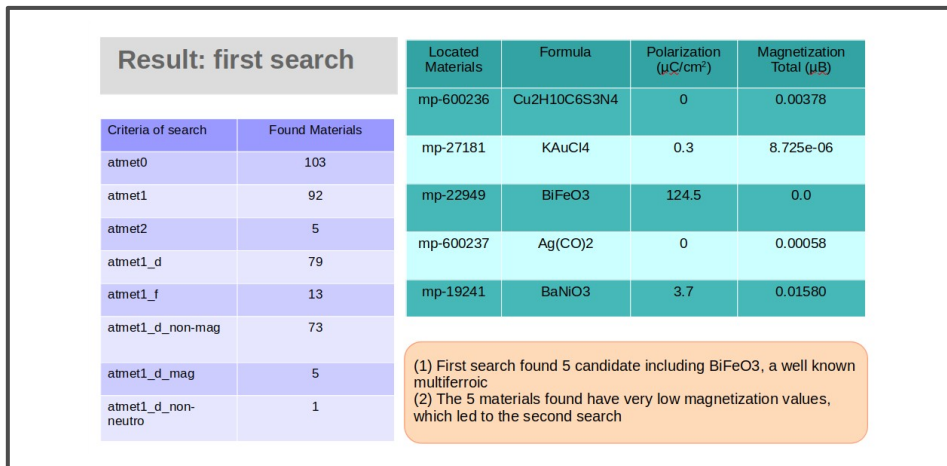
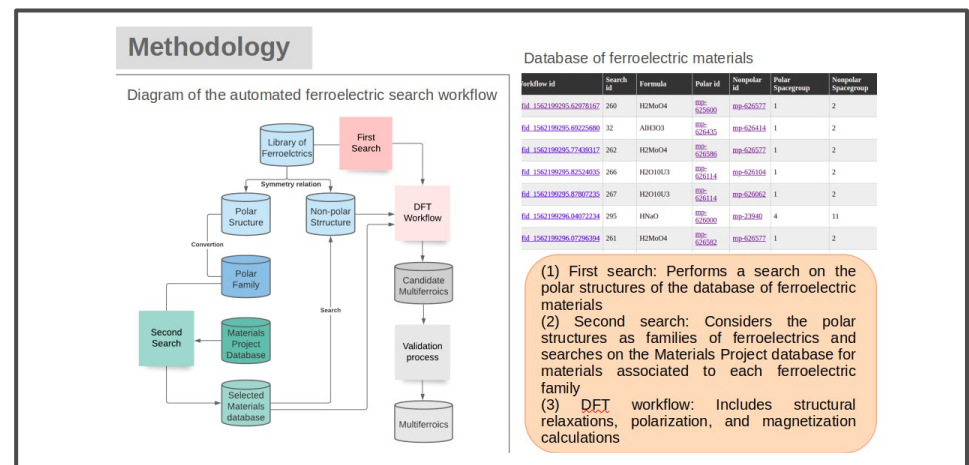
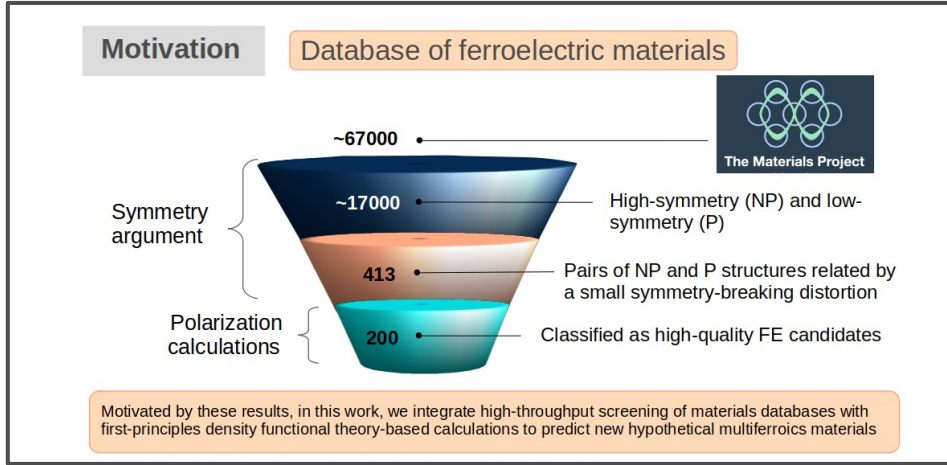
# High-throughput search of multiferroic materials within different families of ferroelectrics

IX WNMESC 2021



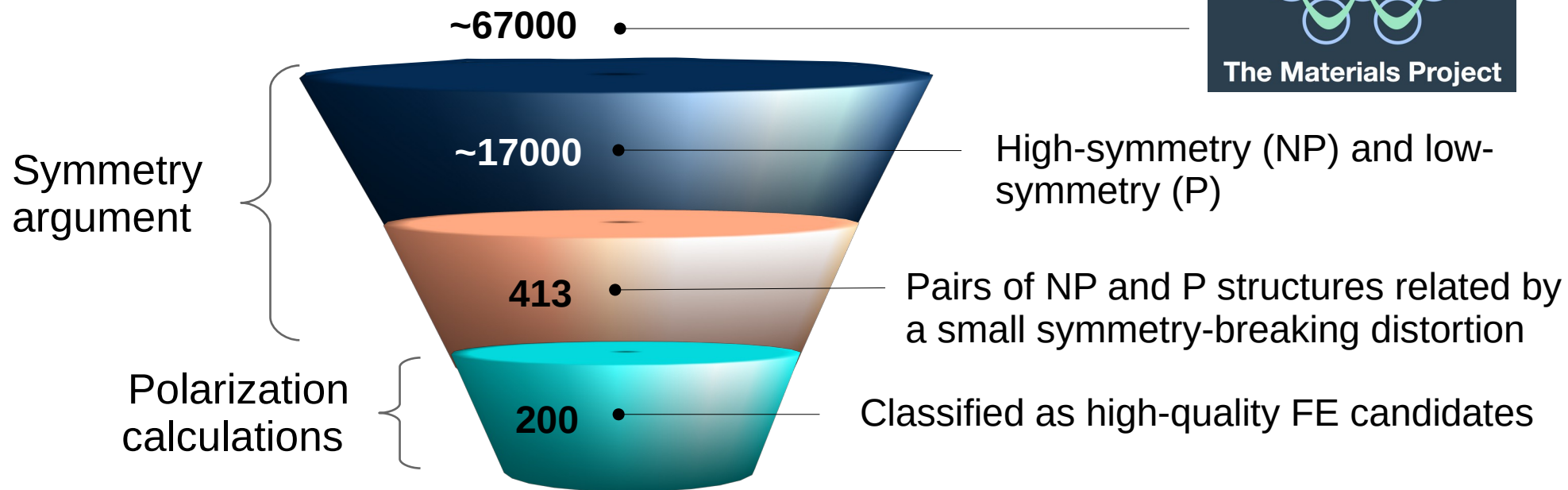
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# Motivation

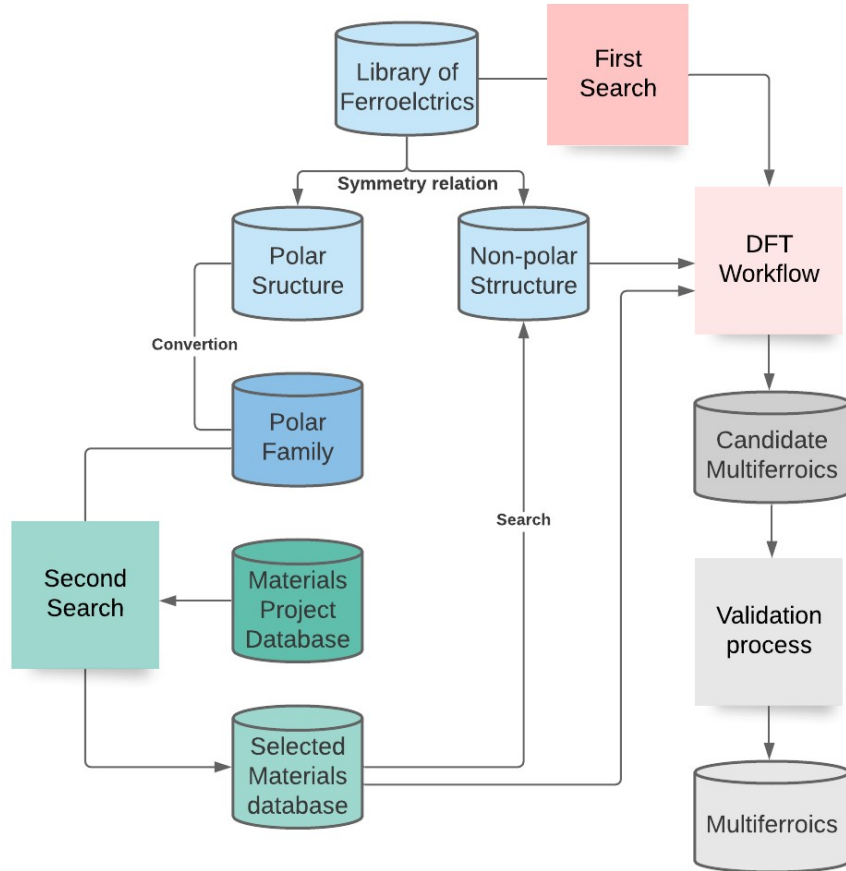
## Database of ferroelectric materials



Motivated by these results, in this work, we integrate high-throughput screening of materials databases with first-principles density functional theory-based calculations to predict new hypothetical multiferroics materials

# Methodology

Diagram of the automated ferroelectric search workflow



Database of ferroelectric materials

orkflow id	Search id	Formula	Polar id	Nonpolar id	Polar Spacegroup	Nonpolar Spacegroup
<a href="#">fid_1562199295.62978167</a>	260	H2MoO4	<a href="#">mp-625600</a>	<a href="#">mp-626577</a>	1	2
<a href="#">fid_1562199295.69225680</a>	32	AlH3O3	<a href="#">mp-626435</a>	<a href="#">mp-626414</a>	1	2
<a href="#">fid_1562199295.77439317</a>	262	H2MoO4	<a href="#">mp-626586</a>	<a href="#">mp-626577</a>	1	2
<a href="#">fid_1562199295.82524035</a>	266	H2O10U3	<a href="#">mp-626114</a>	<a href="#">mp-626104</a>	1	2
<a href="#">fid_1562199295.87807235</a>	267	H2O10U3	<a href="#">mp-626114</a>	<a href="#">mp-626062</a>	1	2
<a href="#">fid_1562199296.04072234</a>	295	HNaO	<a href="#">mp-626000</a>	<a href="#">mp-23940</a>	4	11
<a href="#">fid_1562199296.07296394</a>	261	H2MoO4	<a href="#">mp-626582</a>	<a href="#">mp-626577</a>	1	2

(1) First search: Performs a search on the polar structures of the database of ferroelectric materials

(2) Second search: Considers the polar structures as families of ferroelectrics and searches on the Materials Project database for materials associated to each ferroelectric family

(3) DFT workflow: Includes structural relaxations, polarization, and magnetization calculations

# Result: first search

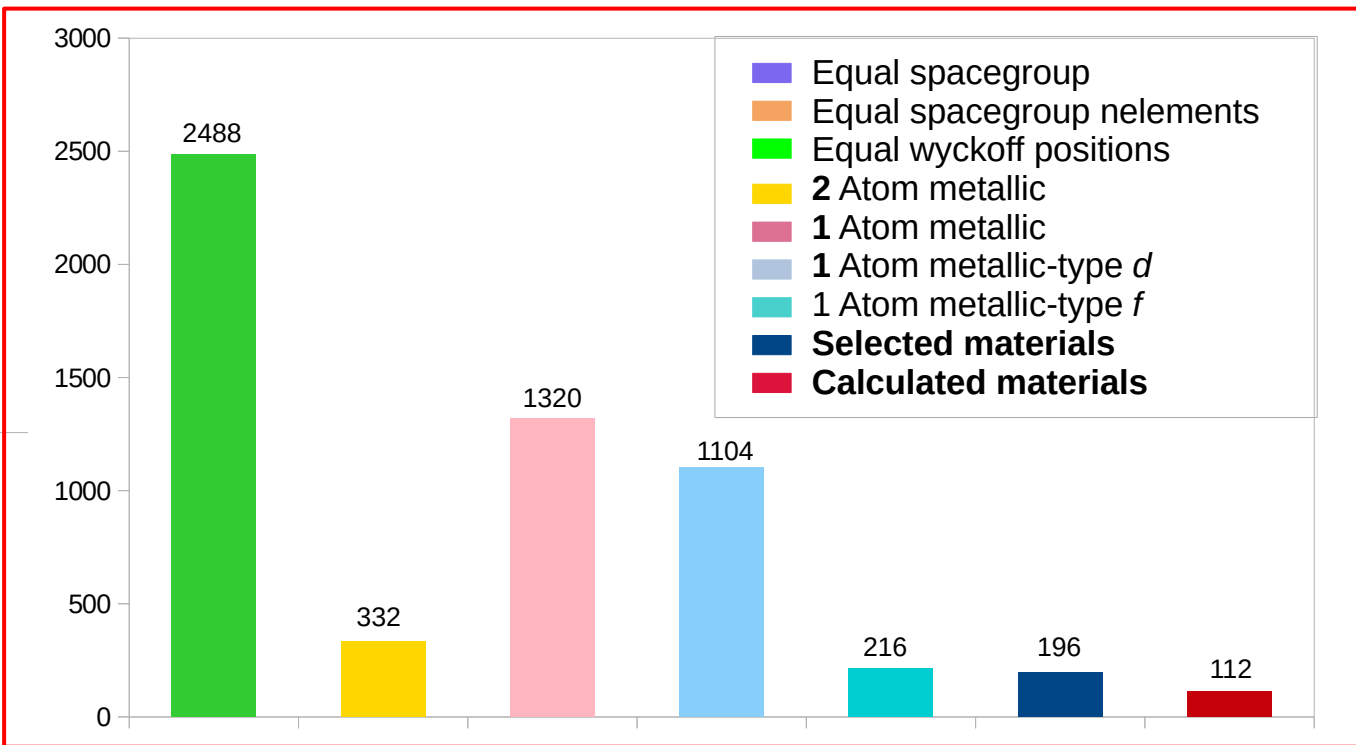
Criteria of search	Found Materials
atmet0	103
atmet1	92
atmet2	5
atmet1_d	79
atmet1_f	13
atmet1_d_non-mag	73
atmet1_d_mag	5
atmet1_d_non-neutro	1

Located Materials	Formula	Polarization ( $\mu\text{C}/\text{cm}^2$ )	Magnetization Total ( $\mu\text{B}$ )
mp-600236	$\text{Cu}_2\text{H}_{10}\text{C}_6\text{S}_3\text{N}_4$	0	0.00378
mp-27181	$\text{KAuCl}_4$	0.3	$8.725\text{e-}06$
mp-22949	$\text{BiFeO}_3$	124.5	0.0
mp-600237	$\text{Ag}(\text{CO})_2$	0	0.00058
mp-19241	$\text{BaNiO}_3$	3.7	0.01580

- (1) First search found 5 candidate including  $\text{BiFeO}_3$ , a well known multiferroic
- (2) The 5 materials found have very low magnetization values, which led to the second search

# Result : second search

(1) Selected materials:  
band gap>0 and  
magnetization>0



## Future Work:

- (1) Investigate specific materials further: different magnetic orders
- (2) Perform DFT calculations using hybrid functionals on new hypothetical multiferroics