Addressing the Materials Genome Initiative through the *aflowlib.org* Consortium

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In this talk we will introduce some of the scientific, technological and computational challenges that we had to solve to create the *aflowlib.org* consortium (a distributed materials properties repository from high-throughput *ab-initio* calculations) [1,2,3]. As examples of application we will introduce results on the search of novel thermoelectrics [4] (Figures 1,2,3), topological insulators [5], and scintillators [6]. If time permits, we will also discuss the search for novel rare-earths-free supermagnets and spintronics materials [7].

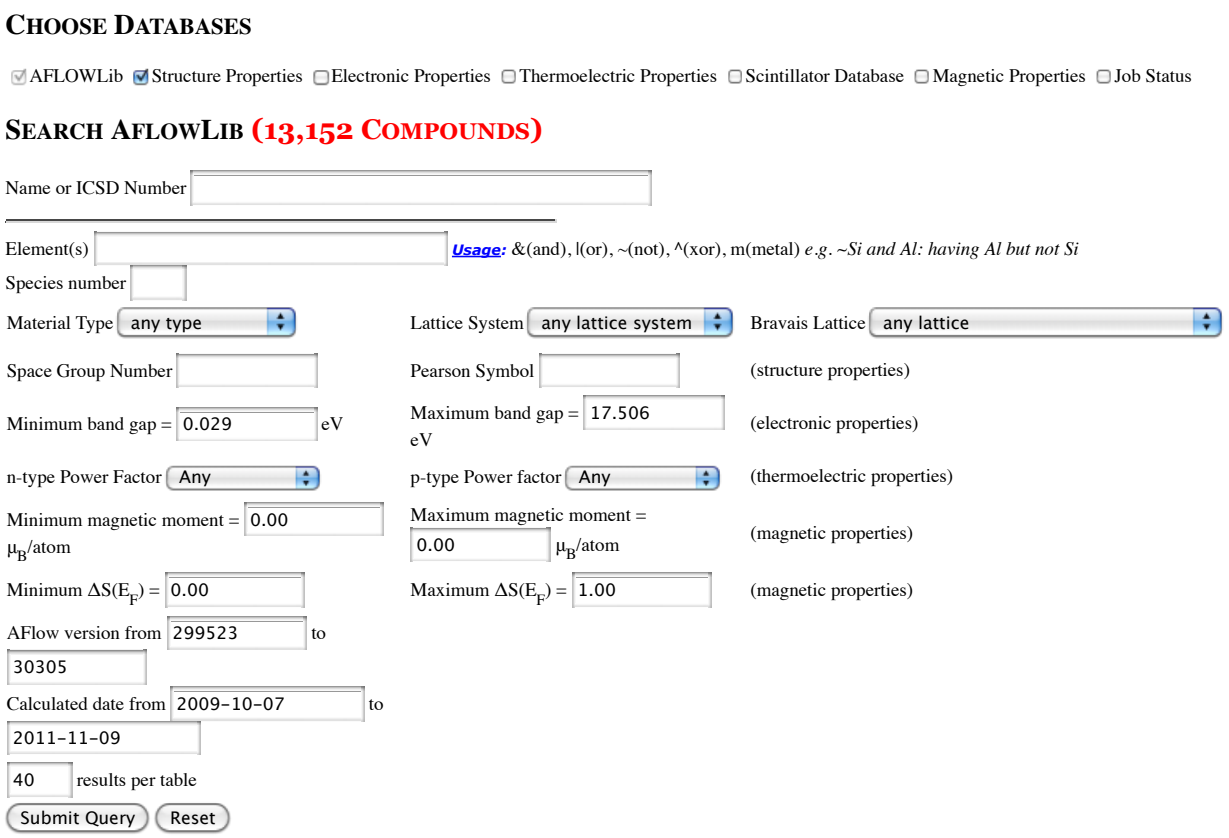

Fig. 1: Example of search in the database. As of March 2012, the user can specify structural, electronic, thermodynamic, and magnetic searches across 15,000+ inorganic compounds, 150,000+ alloy entries, and 50,000+ magnetic and spintronics systems.

30 mm

Index	▲Name [1]	ICSD Number [1]	Bravais Lattice	Number of Atoms	<P_n>/L (μW/cmK²nm) [4]	<P_p>/L (μW/cmK²nm) [4]	S_n (μV/K) [4]	S_p (μV/K) [4]	Prototype Name
1	$F_3Fe_1K_1$	15424	CUB (Cubic)	5	0.15	2.17	-116.36	91.29	F3Fe1K1_ICSD_15424
2	$F_3Fe_1Rb_1$	49586	CUB (Cubic)	5	0.24	1.50	-91.73	91.04	F3Fe1Rb1_ICSD_49586
3	$Fe_1La_1O_3$	29118	CUB (Cubic)	5	0.31	2.00	-139.02	92.92	Fe1La1O3_ICSD_29118

Fig. **2**: Results of a Thermoelectric Properties search within aflowlib.org. From left to right: index, name, ICSD number, Bravais Lattice, Number of Atoms, Relative Power Factors <*P*>/*L* of n- and p-doped nano-sintered compounds, Seebeck coefficients for n- and p-doped cases *(μV/K),* Prototype Name.

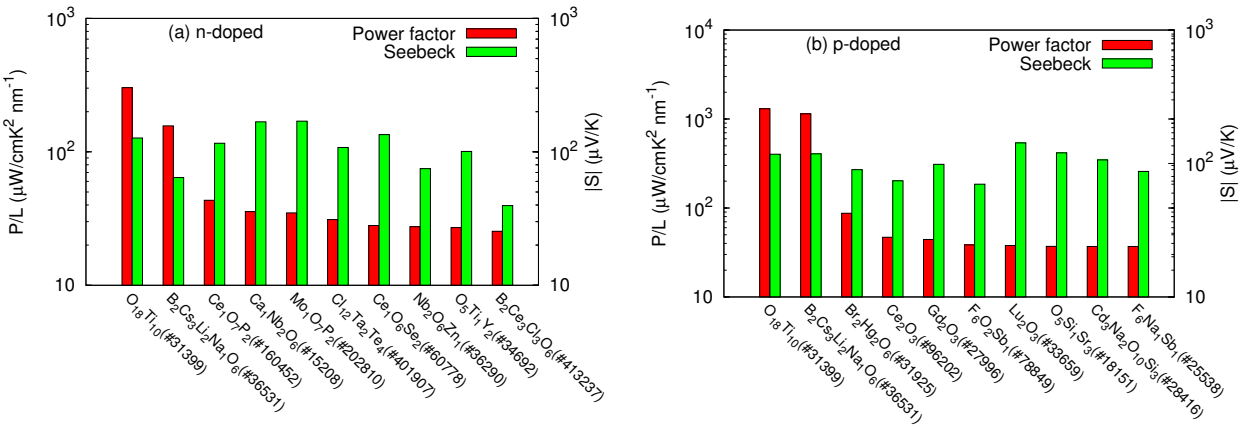

Fig. 3: The best ten (a) n- and (b) p-doped compounds of highest power factor normalized by grain size. The optimal Seebeck coefficients are shown as well.

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