Designing High-Tc Superconductors with BCS-inspired Screening, Density Functional Theory and Deep-learning

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Motivation

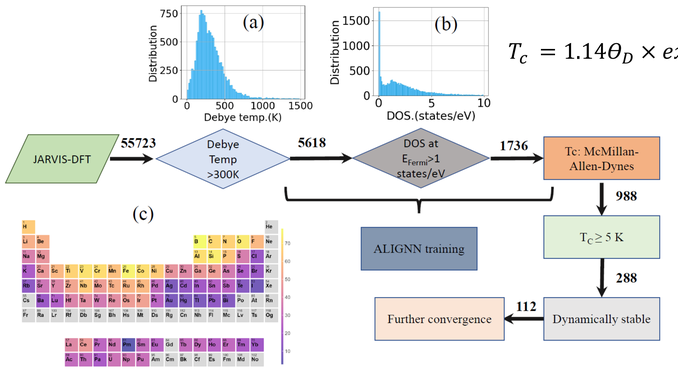
- Identify high-T_C conventional (phonon-mediated) superconductors
- Electron-phonon coupling (EPC) parameter database
- Deep-learning models to predict superconductor properties

Superconductivity

- Materials to conduct electricity without energy loss when they are cooled below a critical temperature, T_C
- MgB_2 (T_C = 39 K): Highest T_C ambient condition conventional superconductor
- High-pressure hydrides for near room-temperature superconductivity such as LaH_{10}, YH_{10}

Workflow

- Using JARVIS-DFT database (55723 materials)
- Debye temperature from elastic tensors (17419)
- Density of states at Fermi-level



DFT Calculations

- Quantum espresso-based Electron-phonon coupling
- T_C calculated with McMillan-Allen-Dynes equation
- Benchmarking using known compounds
- JARVIS-DFT k-points
- At least 2x2x2 q-points
- Broadening & tetrahedron methods

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

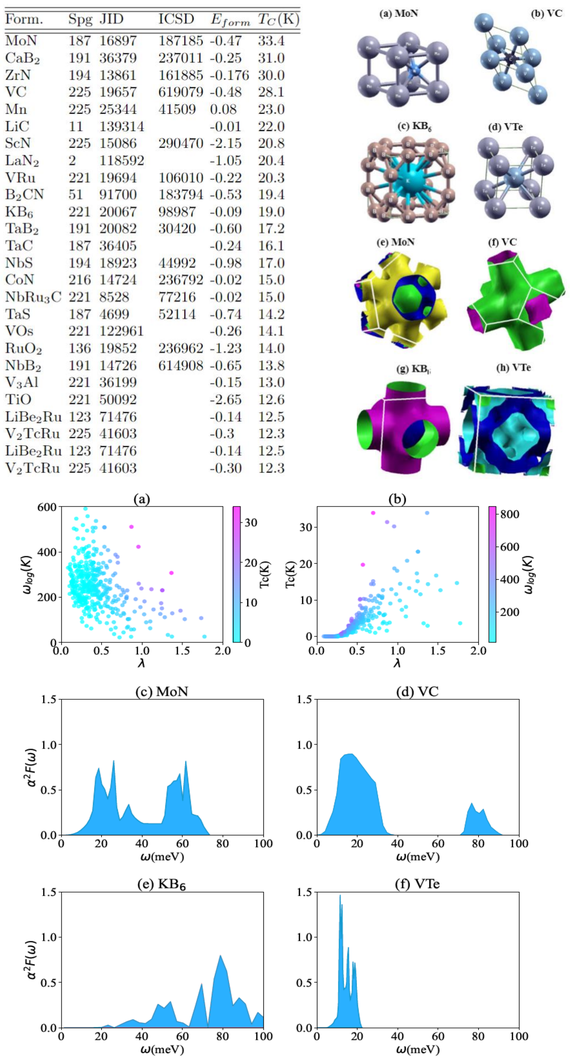
$$T_c = \frac{\omega_{log}}{1.2}\exp[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}]$$

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

Form.	Spg	JID	Exp	SCDFT	LM	J-Scr
Al	225	816	1.2	1.55	0.3	1.6
Ta	229	1014	4.5	5.17	2.45	7.6
Pb	225	961	7.2	6.06	4.95	5.4
Nb	229	934	9.3	10.29	7.0	10.7
ZrN	225	19679	10.0	11.6	6.12	10.0
V_3Si	223	14960	17	18.1	13.1	17.6
MgB_2	191	19821	39	35.4	20.04	33.0
V	229	14837	5.3			18.3
Nb_3Si	223	15938	18.0			16.5
NbO	221	14492	1.38			3.6
NbC	225	19889	12			17.1
NbN	221	36335	16.0			17.6
YB_6	221	20620	7.2			5.1
Nb_3Al	223	11981	16.8			9.0
YH_{10}(250GPa)	225		260			213.5
LaH_{10}(250GPa)	225		211			190.0

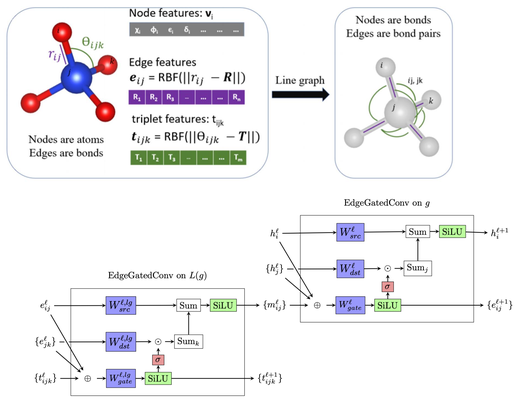
EPC database & candidate mats.

Form.	Spg	JID	ICSD	E_{form}	T_C(K)
MoN	187	16897	187185	-0.47	33.4
CaB_2	191	36379	237011	-0.25	31.0
ZrN	194	13861	161885	-0.176	30.0
VC	225	19657	619079	-0.48	28.1
Mn	225	25344	41509	0.08	23.0
LiC	11	139314		-0.01	22.0
ScN	225	15086	290470	-2.15	20.8
LaN_2	2	118592		-1.05	20.4
VRu	221	19694	106010	-0.22	20.3
B_2CN	51	91700	183794	-0.53	19.4
KB_6	221	20067	98987	-0.09	19.0
TaB_2	191	20082	30420	-0.60	17.2
TaC	187	36405		-0.24	16.1
NbS	194	18923	44992	-0.98	17.0
CoN	216	14724	236792	-0.02	15.0
$NbRu_3C$	221	8528	77216	-0.02	15.0
TaS	187	4699	52114	-0.74	14.2
VOs	221	122961		-0.26	14.1
RuO_2	136	19852	236962	-1.23	14.0
NbB_2	191	14726	614908	-0.65	13.8
V_3Al	221	36199		-0.15	13.0
TiO	221	50092		-2.65	12.6
$LiBe_2Ru$	123	71476		-0.14	12.5
V_2TcRu	225	41603		-0.3	12.3
$LiBe_2Ru$	123	71476		-0.14	12.5
V_2TcRu	225	41603		-0.30	12.3

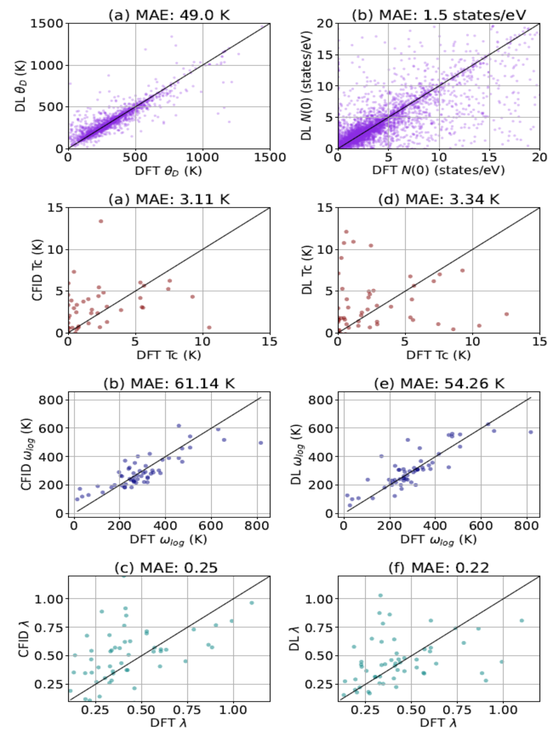


ALIGNN model

- Atomistic line graph neural network model



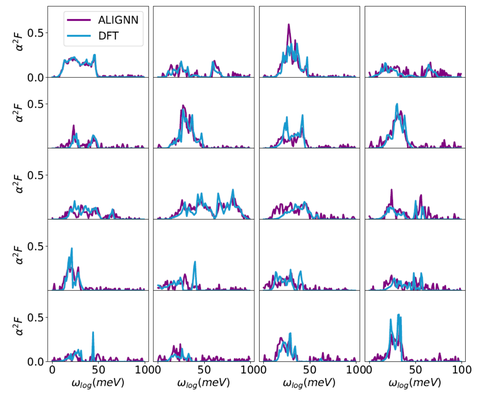
Predicting scalar EPC properties



- 8293 out of 431778 materials in COD database

Predicting Eliashberg function

- 5 % improvement in accuracy than direct predictions



Publications

- "*Designing High-Tc Superconductors with BCS-inspired Screening, Density Functional Theory and Deep-learning,*" arXiv:2205.00060 (2022).
- "*Atomistic Line Graph Neural Network for improved materials property predictions",* npj Computational Materials, 7, 1 (2022).
- "*The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design*", npj Computational Materials, 6, 1 (2020).