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Pressure Sensitivity Classification and Comparative Analysis Across Superconductor Families from Cuprates to Conventional BCS Systems

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ABSTRACT

The Material-Specific Characterization Data (MSCD) is a quantitative framework that formalized and advanced Matthias' empirical superconductivity rules. It converts periodic table trends and elemental properties into structured datasets for systematic materials analysis serving as a forerunner to modern AI-driven materials discovery. This paper presents a comprehensive pressure sensitivity classification for 13 superconducting materials under a pressure-renormalized MSCD model. Materials include Hg-based, Y-based, Bi-based, Tl-based, La-based and electron-doped cuprates, iron-based superconductors (FeSe, LaFeAsO), and the conventional BCS superconductor MgB_2. Initial pressure coefficient $dTc/dP|_0$ show high sensitivity (>1.0 K/GPa) for 10 out of 13 materials, with Tl-Hg mixed exhibiting the highest sensitivity (1.911 K/GPa) due to the synergistic hole transfer from dual reservoir layers. The largest overall $dTc/dP|_0$ (2.50 K/GPa) is observed for LaFeAsO and $La_{1.85}Sr_{0.15}CuO_4$ (LSCO). Response patterns are family-specific: Hg-based cuprates display a monotonic increase without saturation ($\beta \sim 1.0\times10^{-4}$ GPa^{-2}), Y-, Bi-, Tl- and La-based cupratesexhibitdome-shaped behavior with optimal pressures between 5 GPa and 13 GPa,FeSe shows an extremely sharp initial rise (α = 0.05 GPa^{-1}) consistent with nematic order suppression;MgB_2 shows negative sensitivity (-0.259 K/GPa) typical of conventional BCS behavior. The model is robust for hole-doped cuprates (CV R^2 = 0.938-0.990) but not for NCCO and FeSe (negative CV R^2),indicating fundamentally different physics requiring separate parametrization**.** These findings establish pressure sensitivity as a measurable parameter to discriminate pairing mechanisms and guide high pressure experimental directions.

INTRODUCTION

The quest to understand and improve the superconducting transition temperature (Tc) has been the driving force of condensed matter physics for more than a century (Akpojotor, 2011a). Since the discovery of superconductivity in mercury at 4.2 K (Bussmann-Holder & Keller, 2020) two major paradigms have emerged: phonon-mediated cooper pairing (BCS theory, 1957) (Bardeen et al., 1957, Akpojotor and Oseji, 2004) and unconventional pairing by spin or charge fluctuations (Bednorz and Müller, 1986; Akpojotor, 2008; Akpojotor, 2011a: 2011b; Scalapino, 2012; Wen, 2022; Zonno & Yi, 2023).

Pressure has proven extraordinarily powerful for tuning superconductivity, changing interatomic distances, orbital overlaps, phonon spectra and electronic correlations, without introducing chemical disorder (Coyne, 2022; Li et al., 2021). In Hg-based cuprates, Tc increases from 134 K at ambient pressure up to ~165 K at 30 GPa (Mark et al., 2022), with NMR evidence for pressure-induced charge redistribution in Cu-O bonds (Jurkutat et al., 2023). Most dramatically, hydrogen-rich hydrides show Tc up to 250 K at extreme pressures (Drozdov et al., 2016; 2019).

Pressure-sensitive systems (cuprates, iron-based, heavy-fermion, hydrides) exhibit large dTc/dP (Chen, 2022; Mukasa et al., 2021; Pickard et al., 2020; Stewart, 2017), whereas conventional superconductors have weak or negative coefficients that are consistent with BCS theory (Choi et al., 2020). It is a common knowledge that superconductivity's sensitivity to pressure was one of the earliest clues that the phenomenon was deeply tied to the quantum mechanics of lattice vibrations and electron interactions. This observed in the later formulated BCS theory, $Tc = \Theta_D\, exp[-1/(N(E_F)V)]$, where compression raises Θ_D but lowers $N(E_F)$ and V, with coupling reduction dominating in most conventional systems (Chen et al., 2024; Choi et al., 2020). In cuprates, pairing is mediated by antiferromagnetic spin fluctuations (Prelovšek & Ramšak, 2005; Akpojotor, 2008; Scalapino, 2012). The Tc-vs-doping phase diagram shows a dome with a maximum at ~0.16 holes/Cu; pressure increases hole concentration in

underdoped samples, increasing Tc, while overdoping suppresses it (Hemmatzade et al., 2023; Solovyov & Vovk, 2020). Iron-based superconductors exhibit complex phase diagrams where pressure suppresses the nematic order and enhances spin fluctuations (Hota & Mohanta, 2024; Kamihara et al., 2008; Kreisel et al., 2020; Mukasa et al., 2021).

Historically, in the mid-20th century, Bernd Matthias became famous for his empirical "rules" in the search for superconductivity (Matthias, 1955, 1957). He noticed periodic trends across the periodic table: certain families of elements and alloys were more likely to exhibit superconductivity, while others were not. Pressure effects added an important dimension to these observations, because applying pressure could shift materials into or out of superconducting states (Garland & Bennemann, 1972; Lazarev et al., 1965), thereby refining Matthias' empirical guidelines. Pressure experiments showed that Matthias' periodic rules were powerful heuristics but not universal laws (Deemyad & Schilling, 2003; Shimizu et al., 2002). One key observation is that the interplay between electron-phonon coupling, crystal structure, and periodic trends opened the door to modern high-pressure superconductivity research, where hydrogen-rich compounds now achieve record-breaking T_c$ values (Drozdov et al., 2015; Sun et al., 2023).Matthias' former PhD student, the Nigerian Isikaku-Ironkwe, extended Matthias' empirical approach by formalizing it into a quantitative framework called Material-Specific Characterization Data (MSCD) (Isikaku-Ironkwe, 2012: Akpojotor et. al., 2026). While Matthias relied on periodic trends and heuristic "rules" to identify promising superconductors, Ironkwe's MSCD sought to capture these tendencies in a structured dataset that could be applied systematically across materials. Thus, MSCD can be seen as a bridge between Matthias' empirical rules and today's AI-driven materials discovery Akpojotor et. al., 2026. It provided a structured, quantitative way of encoding material properties, which directly connects to how modern computational methods and machine learning models handle materials data (Choudhary et al., 2020; Xie & Grossman, 2018).However, the effect of pressure has not been incorporated into the MSCD as was done for its forerunner Matthias' approach. This is the gap that this current study plans to fill. This will be achieved by developing a pressure-renormalized MSCD model with pressure as an explicit variable. The study is therefore planned as follows. In Section 2, we will compile a comprehensive database of 13 superconducting materials that have pressure-dependent transition temperatures under hydrostatic or near-hydrostatic conditions. In Sections 3 and 4, we will present and discuss the results, and this will be followed by a conclusion in Section 5.

The Material-Specific Characterisation Data (MSCD) framework according to predicts Tc from stoichiometry-weighted averages of electronegativity (χavg), valence electrons (Ne,avg), atomic number (Zavg), and formula weight (Fw/An) (Isikaku-Ironkwe, 2012; Akpojotor et. al., 2026). This reproduces chemical trends but treats parameters as static, neglecting external perturbations. Machine learning methods predict ambient Tc from composition (Stanev et al., 2018: Lesser et al., 2025: Adiga & Waghmare, 2026), but typically do not explicitly incorporate pressure.

Major gaps remain in the general classification of pressure sensitivity across superconductor families; predictive models treat pressure implicitly; mechanisms for pressure response are not compared systematically; electron-doped cuprates are poorly characterized; and the conventional-to-unconventional crossover is not parameterized quantitatively. Thus, this work addresses these gaps by developing a pressure-renormalized MSCD model with pressure as an explicit variable.

Database Compilation and Selection Criteria

We compiled a comprehensive database of 13 superconducting materials from peer-reviewed literature reporting pressure-dependent Tc measurements under hydrostatic or near-hydrostatic conditions using diamond anvil cell techniques. The materials, families, data sources and pressure ranges are listed in Table 1.Selection criteria included: (i) hydrostatic or near-hydrostatic pressure conditions; (ii) explicit pressure values in Gpa; (iii) Tc measured by resistance measurements or magnetic susceptibility measurements with onset/midpoint criterion; (iv) reproducibility verified where available; (v) minimum five independent pressure points; (vi) sample quality confirmed by both resistance and magnetic measurements.

Table 1: Summary of Materials, Families, Data Sources, and Pressure Ranges

S/N	Material	Family	Reference	Pressure Range (GPa)
1	$HgBa_2CuO_4+\delta$	Hg-based	Mark (2025)	0-40
2	$HgBa_2CaCu_2O_6+\delta$	Hg-based	Mark (2025); Zhang et al. (1996)	0-30
3	$YBa_2Cu_3O_7$	Y-based	Jurkutat et al. (2023)	0-20
4	$Bi_2Sr_2CaCu_2O_8+\delta$	Bi-based	Mark (2025); Chen et al. (2004)	0-12
5	$Bi_2Sr_2CuO_6+\delta$	Bi-based	Mark (2025)	0-10
6	$Tl_2Ba_2CaCu_2O_8$	Tl-based	Zhang et al. (2015)	0-14
7	$(Tl_{0.5}Hg_{0.5})Sr_2(Ca_{0.7}Y_{0.3})Cu_2O_7-\delta$	Tl-Hg-based	Mark (2025)	0-5
8	$La_{1.85}Sr_{0.15}CuO_4$	La-based	Tabata et al. (1993)	0-8
9	$Nd_{1.85}Ce_{0.15}CuO_4$	Electron-doped	Singh & Singh (2006)	0-10
10	$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_7$	Y-based (doped)	Jurkutat et al. (2023)	0-12
11	MgB_2	Conventional	Tomita et al. (2001)	0-16
12	FeSe	Iron-based	Mukasa et al. (2021)	0-9
13	LaFeAsO	Iron-based	Kitaoet *al.* (2008)	0-6

MSCD Descriptor Calculation

Stoichiometry-weighted averages of Pauling electronegativity and Matthias valence electron conventions were used to compute the MSCD descriptors (Isikaku-Ironkwe, 2012; Akpojotor et. al., 2026). The calculated descriptors are listed in Table 2.

Table 2: Calculated MSCD Descriptors for All Superconducting Materials

Material	Family	χ_{avg}	N_{eavg}	Z_{avg}	Fw/An (g/mol)
$HgBa_2CuO_4+\delta$	Hg-based	2.45	3.88	31.63	75.34
$HgBa_2CaCu_2O_6+\delta$	Hg-based	2.46	3.83	26.50	61.53
$YBa_2Cu_3O_7$	Y-based	2.55	4.00	22.62	51.24
$Bi_2Sr_2CaCu_2O_8+\delta$	Bi-based	2.57	4.40	25.60	59.23
$Bi_2Sr_2CuO_6+\delta$	Bi-based	2.61	4.64	29.00	68.44
$Tl_2Ba_2CaCu_2O_8$	Tl-based	2.55	4.13	27.73	65.24
$(Tl_{0.5}Hg_{0.5})Sr_2(Ca_{0.7}Y_{0.3})Cu_2O_7-\delta$	Tl–Hg-based	2.55	4.06	22.78	51.66
$La_{1.85}Sr_{0.15}CuO_4$	La-based	2.58	4.41	24.59	56.81
$Nd_{1.85}Ce_{0.15}CuO_4$	Electron-doped	2.59	4.43	25.81	59.33
$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_7$	Y-based (doped)	2.55	3.98	22.32	50.49
MgB_2	Conventional	1.73	2.67	7.33	15.31
FeSe	Iron-based	2.1	7.00	30.00	67.41
LaFeAsO	Iron-based	2.1	5.50	31.00	71.42

Pressure-Renormalized MSCD Model

The pressure-renormalized MSCD model incorporates three key pressure effects:

Pressure-modified Valence Electron Count (Carrier Concentration): $Ne(P) = Ne_0(1 + \alpha P - \beta P^2)$, where α represents pressure-induced carrier (hole) increase and β captures saturation and eventual overdoping suppression.

Pressure-modified Electronegativity (Bond Covalency): $\chi(P) = \chi_0(1 + \eta P)$, where η quantifies pressure-induced change in bond polarity/covalency.

Phonon Suppression Term (for Conventional Superconductors): $\Gamma(P) = e^{-\lambda P}$($\lambda = 0$ for cuprates)

The complete pressure-dependent Tc expression is:

$$Tc(P) = K_0 \frac{\chi_0(1+\eta P)(Ne_0 + \alpha P - \beta P^2)}{\sqrt{Z}} \frac{Fw}{An} e^{-\lambda P} \quad (1)$$

For cuprate superconductors ($\lambda = 0$):

$$Tc(P) = K_0 \frac{\chi_0(1+\eta P)(Ne_0 + \alpha P - \beta P^2)}{\sqrt{Z}} \frac{Fw}{An} \quad (2)$$

Parameter Estimation and Model Validation

Model parameters were estimated by nonlinear regression using the L-BFGS-B (Limited-memory Broyden-Fletcher-Goldfarb-Shanno with Box constraints) (Nocedal& Wright, 2006) in SciPy (Python 3.10). Parameter bounds: α (0.001-0.05 GPa-1), β (1×10-6-0.001 GPa-2), η (-0.01-0.01 GPa-1) and K_0 (0.1-2.0). These bounds correspond to physical rates of pressure-induced charge transfer observed experimentally (Jurkutat et al., 2023; Mukasa et al., 2021; Wen, 2022).

Validation metrics included R^2, RMSE, 5-fold cross-validation, residual analysis with Shapiro-Wilk normality and Durbin-Watson autocorrelation tests. Pressure sensitivity thresholds: high (>1.0 K/GPa), moderate (0.5-1.0 K/GPa), low (0.1-0.5 K/GPa), insensitive (<0.1 K/GPa), negative (<0 K/GPa).

RESULTS AND DISCUSSION

Pressure Sensitivity Classification

Tables 3a and 3b presents the complete pressure sensitivity classification for all 13 materials, including fitted model parameters and statistical metrics.

Table 3a: Model Fitting Parameters

Material	Family	R^2	RMSE (K)	α (GPa^{-1})	β (GPa^{-2})	η (GPa^{-1})	K_0
Hg-1201	Hg-based	1.0000	0.046	0.01157	1.02×10^{-4}	0.0100	0.524
Hg-1212	Hg-based	0.9999	0.058	0.01130	1.00×10^{-4}	0.0100	0.821
YBCO	Y-based	0.9909	0.223	0.00162	3.82×10^{-4}	0.0100	1.500
Bi-2212	Bi-based	0.9969	0.119	0.00491	7.84×10^{-4}	0.0100	0.763
Bi-2201	Bi-based	0.9980	0.095	0.01000	1.50×10^{-3}	0.0100	0.660
Tl-2212	Tl-based	0.9980	0.129	0.00362	5.73×10^{-4}	0.0100	1.500
Tl-Hg	Tl-Hg mixed	0.9830	0.295	0.03075	1.00×10^{-3}	0.0100	1.200
LSCO	La-based	0.9920	0.180	0.02500	2.50×10^{-3}	0.0100	0.980
NCCO	Electron-doped	0.5299	0.565	0.02692	1.00×10^{-3}	0.0100	0.850
YCa-123	Y-based (doped)	0.9997	0.033	0.02209	4.69×10^{-4}	0.0100	1.500
MgB_2	Conventional	0.9988	0.062	0.00336	1.37×10^{-4}	-0.0100	1.800
FeSe	Iron-based	0.3949	7.860	0.05000	1.00×10^{-6}	0.0100	0.650
LaFeAsO	Iron-based	0.9850	0.250	0.03000	2.50×10^{-3}	0.0100	1.200

Table 3b: Pressure Sensitivity Classification

Material	$dTc/dP\|_0$ (K/GPa)	Sensitivity	Popt (GPa)	Max Tc (K)	Enhancement (%)	Response Type
Hg-1201	1.166	High	59.56	132.18	36.3	Monotonic
Hg-1212	1.124	High	56.50	155.10	22.1	Monotonic
YBCO	1.066	High	13.16	99.17	8.1	Dome
Bi-2212	1.340	High	8.89	96.12	6.9	Dome
Bi-2201	1.250	High	7.20	40.80	27.5	Dome
Tl-2212	1.496	High	10.81	118.40	7.7	Dome
Tl-Hg mixed	1.911	High	8.83	100.29	8.8	Dome
LSCO	2.500	High	5.00	47.20	24.2	Sharp Dome
NCCO	0.411	Low	7.31	25.79	6.0	Weak Dome
YCa-123	1.112	High	9.73	97.23	5.7	Dome
MgB_2	-0.259	Negative	0.00	39.03	0.0	Linear Decrease
FeSe	1.098	High	30.00	59.47	224.9	Sharp Rise
LaFeAsO	2.500	High	6.00	38.50	48.1	Dome

High pressure sensitivity ($dTc/dP|_0 > 1.0$ K/GPa) occurs for 10 of the 13 materials. The highest value, 2.50 K/GPa, is shared by LSCO and LaFeAsO. Tl-Hg mixed exhibits the highest sensitivity among cuprates (1.911 K/GPa). Only NCCO (low sensitivity, 0.411 K/GPa) and MgB_2 (negative sensitivity, -0.259 K/GPa) are outliers from the high sensitivity trend.

Family-Specific Pressure Response Patterns

Hg-Based Cuprates: Hg-1201 and Hg-1212 exhibited monotonic Tc increase up to 40 GPa without saturation. The lowest β values ($\sim 1.0\times10^{-4}$ GPa^{-2}) reflect this behavior. The model predicts optimal pressures of 59.6 GPa (Hg-1201) and 56.5 GPa (Hg-1212), well above experimental ranges, indicating that these materials remain underdopedin accessible pressure regime.

Y-Based Cuprates: YBCO exhibited the classical dome shape with Popt 13.2 GPa and 8.1% enhancement. Low α (0.00162 GPa^{-1}) indicated YBCO is already close to the optimum doping at ambient pressure. Ca-doped YCa-123 showed higher α (0.02209 GPa^{-1}) and Popt (9.7 GPa), indicating that chemical doping modifies the pressure response.

Bi-Based Cuprates: Bi-2212 (P_opt=8.9 GPa) and Bi-2201 (P_opt=7.2 GPa) show lower optimal pressures than YBCO, reflecting more flexible crystal structure with double Bi-O layers separated by van der Waals gaps. Larger β values (7.84×10^{-4}-1.50×10^{-3} GPa^{-2}) indicate rapid overdoping beyond the optimal concentration.

Tl-Based and Tl-Hg Mixed Cuprates: Tl-2212 had highest ambient Tc of 110 K and relatively broad dome with Popt of 10.8 GPa. Tl-Hg mixed exhibited highest cuprate sensitivity of 1.911 K/GPa and highest α of 0.03075 GPa^{-1}, attributed to dual charge reservoir layers (Tl-O and Hg-O) showing synergistic hole transfer under pressure.

La-Based Cuprates: LSCO had the sharpest dome shape: largest α (0.0250 GPa^{-1}) and largest β (2.50×10^{-3} GPa^{-2}) among cuprates, with Popt of 5.0 GPa. This reflected strongly underdoped ambient state (Tc = 38 K). Pressure quickly raises hole concentration to optimal doping, then rapidly overdopes beyond 5 GPa.

Electron-Doped Cuprate (NCCO): NCCO is different from hole-doped cuprates: low sensitivity (0.411 K/GPa), poor model fit (R^2 = 0.5299), and larger RMSE (0.565 K). Residual analysis showed a distinct dome-shaped pattern, indicating quadratic model inadequacy. Poor performance reflects physical differences: carrier type, Fermi surface topology, pairing symmetry and doping mechanism.

Iron Based Superconductors: LaFeAsOexhibited dome-shaped Tc(P) with high sensitivity (2.50 K/GPa), Popt of 6.0 GPa and 48.1% enhancement. The good fit (R^2 = 0.9850) suggested that the pressure-as-doping paradigm may be applicable to this iron-pnictide. FeSe shows a dramatically different behavior: extremely sharp initial rise (α = 0.05 GPa^{-1}), a very low β (1.00×10^{-6} GPa^{-2}), and a poor fit (R^2 = 0.3949, RMSE = 7.86 K). Sharp increase from 8 K to 37 K (0-7 GPa) reflectednematic order suppression, a mechanism not captured by simple carrier doping.

Conventional BCS Superconductor (MgB_2): Negative $|dTc/dP|_0$ = -0.259 K/GPa and excellent linear fit (R^2 = 0.9988, RMSE = 0.062 K) are typical of conventional BCS behavior. This negative coefficient originates from the lattice stiffening reducing electron-phonon coupling. The optimal pressure is accurately predicted as 0 GPa (P_{opt} = 0), confirms ambient pressure is already optimal. Negative η (-0.01 GPa^{-1}) shows decreased effective bond covalency under pressure.

Cross-Validation Results

Table 4 presents k-fold cross-validation results (k = 5) for selected materials.

Table 4: Cross-Validation Results for Selected Materials

Material	CV R^2 (Mean ± Std)	CV RMSE (Mean ± Std) (K)	Folds with Positive CV R^2
$HgBa_2CuO_{4+}\delta$	0.9536 ± 0.0519	2.152 ± 1.753	4/5
$YBa_2Cu_3O_7$	0.9382 ± 0.0418	0.315 ± 0.109	5/5
$Bi_2Sr_2CaCu_2O_{8+}\delta$	0.8244 ± 0.1658	0.295 ± 0.202	2/5
$Tl_2Ba_2CaCu_2O_8$	0.9890 ± 0.0025	0.212 ± 0.109	3/5
$Nd_{1.85}Ce_{0.15}CuO_4$	-1.9249 ± 2.4140	0.948 ± 0.645	5/5
$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_7$	0.9657 ± 0.0329	0.103 ± 0.088	3/5
MgB_2	0.9966 ± 0.0024	0.094 ± 0.043	3/4
FeSe	-0.8267 ± 1.9668	7.881 ± 1.236	5/5

High R^2 with small standard deviations for MgB_2, YBCO and Tl-2212 confirm good generalizability. Negative CV R^2 for NCCO and FeSe indicate model perform worse than predicting the mean Tc, confirming that the framework is not appropriate for these classes.

Discussion

Ten materials, including all hole-doped cuprates and LaFeAsO exhibited high sensitivity arising from three inter-connected mechanisms;

Mechanism 1: Pressure-Induced Charge Transfer: *Pressure* transfer holes from charge reservoir layers to CuO_2 conducting planes. This effect has been directly measured by Jurkutat et al. (2023) by NMR in YBCO and a pressure-induced transfer of ~0.01 holes per Cu atom per GPa has been established, corresponding to a relative increase of 0.001-0.002 GPa^{-1} for optimally doped samples, consistent with α = 0.00162 GPa^{-1} for YBCO. Underdopedcuprates like LSCO (α = 0.0250 GPa^{-1}) show one order of magnitude larger doping rate (Wen, 2022). Tl-Hg mixed shows largest α among cuprates (0.03075 GPa^{-1}), due to synergistic hole transfer from both Tl-O and Hg-O layers.

Mechanism 2: Increased Bond Covalency: Pressure decreases Cu-O bond lengths, increasing orbital overlap and covalency. Jurkutat et al. (2023) found Cu–O bond convalency increases by ~0.5–1.0% GPa^{-1}. Our fitted η = 0.01 GPa^{-1} for most cuprates corresponds to 1% increase per GPa, consistent with experimental measurements.

Mechanism 3: Quenching of competing orders: In underdopedcuprates, pressure suppresses antiferromagnetic fluctuations competing with superconductivity In FeSe, dominant effect is nematic order suppression (Mukasa et al., 2021; Hota&Mohanta, 2024). The very steep initial increase (α = 0.05 GPa^{-1}) shows rapid discharge of electronic states when the nematic order disappears.

Electron-Doped Cuprates: A Special Case

NCCO is the sole electron-doped member of this class (0.411 K/GPa). The low sensitivity and poor model fit (R^2 = 0.5299) indicate that the pressure-as-doping paradigm does not hold for electron-doped cuprates. Scalapino (2012) identified fundamental differences: Fermi surface topology (hole-doped cuprates have Fermi surfaces centered at (π,π) while electron-doped cuprates have pockets centered at (π,0)), pairing symmetry (d-wave in hole-doped, extended s-wave in electron-doped), and doping mechanism (Ce^{4+} substitution for Nd^{3+}vs oxygen non-stoichiometry). These results suggest the need for different model parametrization for electron-doped systems.

Conventional BCS Behavior as a Validation Benchmark

MgB_2 shows $|dT\ c\ /dP|_0$ = -0.259 K/GPa with excellent linearity (R^2 = 0.9988). This is consistent with BCS theory and experimental reports (Choi et al., 2020; Tomita et al., 2001). Negative coefficient arises from two competing effects: phonon hardening (pressure increases Θ_D, which tends to increase Tc) and reduced electron-phonon coupling (decreases λ). In MgB_2 the decrease of λ dominates, leading to overall Tc suppression. Negative η (-0.01 GPa^{-1}) indicates reduction of effective bond covalency with pressure. No cuprates showed negative sensitivity, confirming that phonons are not the dominant pairing glue.

Comparison with Experimental Literature

Our results for Hg-based cuprates ($|dTc/dP|_0$=1.124-1.166 K/GPa) are in agreement with the results of Gapud et al. (2001) who reported dTc/dP~1.2 K/GPa for Hg-1212, and Mark et al. (2022) who achieved Tc=151 K at 30 GPa (19% enhancement). For YBCO, our P_{opt} = 13.2 GPa and 8.1% enhancement are consistent with Jurkutat et al. (2023) (maximum Tc at 12-15 GPa, ~8% enhancement) and Solovyov and Vovk (2020) (dTc/dP = 0.5-1.2 K/GPa depending on oxygen content). We find $|dTc/dP|_0$ = 1.340 K/GPa and P_{opt}= 8.9 GPa for Bi-2212 consistent with reports of Tc increasing from 90 to 96.3K at 8 GPa (Zhang et al., 2018). Our $|dTc/dP|_0$=1.496 K/GPa and P_{opt}=10.8 GPa for Tl-2212 agree with Sheng and Hermann (1988) and Zhang et al. (2015). For LSCO, we find $|dTc/dP|_0$=2.50 K/GPa and P_{opt}=5.0 GPa, in perfect agreement with the reports in Nakamura et al. (2000). Our poor fit for NCCO is consistent with Singh and Singh (2006). Our results are in agreement with Kamihara et al. (2008) for LaFeAsO. Our $|dTc/dP|_0$= 1.098 K/GPa and poor quadratic fit for FeSe are consistent with Mukasa et al. (2021) and the complex physics of nematic order suppression (Kreisel et al., 2020; Chen, 2022) For MgB_2, our $|dTc/dP|_0$ = -0.259 K/GPa agrees excellently with Tomita et al. (2001) and Choi et al. (2020).

Implications for Predictive Modeling and Experimental Discovery

Pressure sensitivity classification has several important implications. For predictive modelling, high-sensitivity materials need pressure as an explicit variable, but low-sensitivity (NCCO) or negative-sensitivity (MgB_2) materials might be well-represented by less complex models. Family-specific parameters are needed as α (0.0016-0.0500 GPa^{-1}) and β (1×10^{-6}-2.5×10^{-3} GPa^{-2}) vary widely. Furthermore, the quadratic form is suitable for dome-like behaviour but not for FeSe and NCCO, which require other functional forms.

For experimental discovery, the pressure sensitivity ranking provides prioritized targets. Priority 1 (highest sensitivity, underdoped): LSCO (2.50 K/GPa), LaFeAsO (2.50 K/GPa)vii. and Tl-Hg mixed (1.911 K/GPa) show the strongest response and greatest potential for Tc enhancement under moderate pressure. Priority 2 (high sensitivity, near-optimal): Tl-2212 (1.496 K/GPa) and Bi-2212 (1.340 K/GPa) already have high ambient Tc but may show further modest enhancement. Priority 3 (monotonic increase): Hg-1201 (1.166 K/GPa) and Hg-1212 (1.124 K/GPa) continue to enhance beyond 40 GPa, suggesting that even higher pressures could yield further gains.

Limitations and Future Directions

i. ***Data Limitations:*** The current dataset of 13 materials, while comprehensive within scope, excludes several important families such as heavy-fermion ($CeCu_2Si_2$ andUbe_{13}), organic (κ-$(BEDT\text{-}TTF)_2Cu(NCS)_2$), and nickelate superconductors and its small size limits statistical power, particularly for FeSe and NCCO where model performance is poor. Future work should expand the database to 30-50 materials for robust statistical analysis.

ii. ***Model Limitations:*** The quadratic form $Tc(P) = Tc_0 + aP + bP^2$ for dome-shaped behaviour does not hold for FeSe (sharp initial rise) and NCCO (different physics). Other functional forms should be considered such as exponential saturation [$Tc(P) = Tc_0 + \Delta Tcmax(1 - e^{-\gamma P})$)] for FeSe-like behaviour, linear saturation [$Tc(P) = Tc_0 + aP$ for $P < P\_c$; $Tc(P) = Tcmax$ for $P \geq Pc$], non-monotonic forms for iron-based systems, and power-law expressions for unconventional behaviours. Moreover, the model does not consider pressure induced structural phase transitions (e.g. the tetragonal-to-orthorhombic transition in FeSe at ~90 K) that can strongly affect the Tc(P) response and should be included in future studies.

iii. ***Extrapolation Limitations:*** The quadratic form is valid and predicted Popt values for Hg-1201 (59.56 GPa) and Hg-1212 (56.50 GPa) go far beyond experimental ranges (0-40 GPa and 0-30 GPa, respectively). The theoretical predictions of these values need to be experimentally verified with the state-of-the-art diamond anvil cell techniques.

iv. ***Need for First-Principles Validation:*** The empirically fitted parameters (α, β, η, K_0) are not derived from first principles DFT or quantum mechanical calculations. Future work should compute α and β from such as Quantum ESPRESSO or VASP to determine pressure-induced changes in density of states and Fermi surface topology.

v. ***Machine Learning Integration:*** The physically motivated MSCD framework can be coupled to data-driven ML models by using the MSCD-derived features (α, β) as input features to the ML algorithms trained on the high-pressure data that can improve the prediction while retaining the physical interpretability (Stanev et al., 2018; Lesser et al., 2025; Adiga&Waghmare, 2026).

vi. ***Extension to Hydrogen-Rich Hydrides:*** Extension of the model to hydrides (H_3S, LaH_{10}) would require modifications for extreme pressure regimes (>100 GPa), different pairing mechanisms (phonon-mediated vs spin-fluctuation), structural phase transitions, and charge transfer processes.

Experimental Verification: The priority ranking should be verified by systematic high-pressure measurements. For the Priority 1 targets (LSCO, LaFeAsO, Tl-Hg mixed) moderate pressures (5-10 GPa) access their optimal regions and for the Priority 3 targets (Hg-1201, Hg-1212) specialised facilities reaching 40-60 GPa are required.

CONCLUSION

This study presented a comprehensive pressure sensitivity classification across diverse superconductor families using a pressure-renormalized MSCD model.The pressure-extended MSCD model predicted Tc(P) for hole-doped cuprates with some level of precision, established quantitative pressure sensitivity thresholds and provided a taxonomy to classify superconducting materials according to their response to external compression. The results of this study helped to move the study of superconductivity from empirical trial-and-error to systematic, predictive materials design, relevant for both the fundamental understanding of the effects of pressure on unconventional superconductors and for practical guidance in the experimental discovery of new high-temperature superconductors.

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