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Review Article

Pd_2ZrIn Heusler Superconductor: Structural Disorder, Electronic Structure, Superconducting Ground State, and First-Principles Research Gaps - A Review

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ABSTRACT
The full-Heusler compound Pd2ZrIn (space group Fm3̄m, No. 225) belongs to a family of palladium-based Heusler superconductors alongside Pd2ZrAl, Pd2HfAl, and Pd2HfIn whose occurrence of superconductivity was originally predicted from electronic-structure calculations and subsequently confirmed by resistivity and magnetic-susceptibility measurements. This review synthesizes the currently available experimental and first-principles literature on Pd2ZrIn, covering its crystal structure and characteristic B2-type antisite disorder, the van Hove scenario invoked to rationalize its occurrence of superconductivity, and the detailed superconducting ground state recently established by muon spin relaxation and rotation (μSR) measurements namely bulk type-II superconductivity with Tc ≈ 2.2 K, a fully gapped, nodeless s-wave order parameter [Δ(0) ≈ 0.33 meV], and preserved time-reversal symmetry. Pd2ZrIn is placed in the broader context of the valence-electron-count (VEC) systematics that organize known Heusler superconductors, and is compared with isostructural and closely related compounds (Pd2ZrAl, Pd2HfAl, ZrPd2Sn, LiPd2Si, MgPd2Sb, ScAu2Al). Although the original 2009 work included electronic-structure calculations for the $Pd_2ZrAl/Pd_2HfAl/Pd_2ZrIn/Pd_2HfIn$ family, the literature located for this review does not provide a dedicated, comprehensive Pd_2ZrIn-specific first-principles treatment of its equilibrium structural parameters, elastic/mechanical response, disorder-dependent electronic structure, phonon dispersion, Eliashberg spectral function $\alpha^2F(\omega)$, and ab initio electron–phonon coupling. These quantities therefore remain well-defined targets for a focused DFT/DFPT investigation. This review identifies these gaps and outlines a computational framework by which they could be addressed.

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INTRODUCTION

In 1903, Fritz Heusler reported that the alloy Mn2CuAl was ferromagnetic despite containing no ferromagnetic element in isolation (Heusler, 1903). This observation gave its name to what has become one of the most populous families of ternary intermetallic structure types, with well over a thousand reported compounds (Graf et al., 2011; Dshemuchadse & Steurer, 2015). Full Heusler compounds crystallize with the general formula XY2Z in the cubic L21 structure (space group Fm3̄m, No. 225), which can be

described as a CaF2-type (fluorite) Y2Z sublattice with the Y atoms forming a cubic cage, also with the X atoms filling the tetrahedral voids (Graf et al., 2011; Górnicka et al., 2024). X and Y are typically transition metals, while Z is a main-group element; in some compounds, as in the present case, X is instead an early transition metal (Zr) and Y a late-transition-metal cage former (Pd), with Z a post-transition metal (In). The diversity of chemistries accessible within this single structural motif underlies the correspondingly diverse physical behaviour reported across the family, including half-metallic ferromagnetism, heavy-fermion behaviour, shape-memory and magnetocaloric effects, and the focus of this review to superconductivity (Graf et al., 2011; Górnicka et al., 2024).

Superconductivity in Heusler Compounds

Superconductivity was first reported in ternary Heusler intermetallics in the early 1980s, and has since been confirmed in more than thirty full-Heusler phases (Klimczuk et al., 2012; Górnicka et al., 2024). A recurring structural motif among the great majority of these superconductors is a cubic cage built from a late d-block metal such as Ni, Pd, Pt, or Au interacting with an electropositive early transition metal or lanthanide and a p-block element; only a small number of Heusler superconductors (e.g., LiGa2Rh, LiGa2Ir) instead build their cage from p-block atoms (Górnicka et al., 2024; Górnicka et al., 2021; Carnicom et al., 2019). Systematic surveys show that nearly all known Heusler superconductors have a valence electron count (VEC) of 25–29, with a strong clustering at VEC = 27 which is close to a maximum in Matthias' empirical Tc–VEC relationship for elemental superconductors and their alloys (Górnicka et al., 2024; Matthias, 1955). Within this VEC window, the highest transition temperatures reported to date belong to ScAu2Al (Tc = 5.12 K, with a record electron-phonon coupling constant $\lambda = 1.25$ among Heuslers) (Kuderowicz & Wiendlocha, 2023) and YPd2Sn (Klimczuk et al., 2012). The pairing mechanism established across the family is conventional, phonon-mediated (BCS) superconductivity, with coupling strengths ranging from weakly coupled (e.g., LiPd2Si, $\lambda = 0.49$ (Górnicka et al., 2024)) to strongly coupled (ScAu2Al (Kuderowicz & Wiendlocha, 2023)). A recurring theoretical ingredient in rationalizing the occurrence and in several cases the magnitude of Tc in these compounds is the van Hove scenario: band-structure calculations reveal saddle points (van Hove singularities) at or near the Brillouin-zone L point, producing a local maximum in the electronic density of states (DOS) at or close to the Fermi level that favours Cooper pairing even under otherwise weak electron-phonon coupling (Winterlik et al., 2009).

Pd-Based Heusler Superconductors and the Discovery of Pd_2ZrIn

The specific subfamily of interest here are the full-Heusler compounds built from a Pd cubic cage combined with an early transition metal (Zr, Hf) and a triel element (Al, In) that was established by Winterlik, Fecher, Thomas, and Felser, who reported four new Heusler superconductors in a single 2009 study: Pd2ZrAl, Pd2HfAl, Pd2ZrIn, and Pd2HfIn (Winterlik et al., 2009). Resistivity measurements placed the superconducting transition temperatures of this group of compounds in the range $T_c \approx 2.4–3.8$ K, with magnetic-field-dependence measurements confirming type-II bulk superconductivity in all four (Winterlik et al., 2009). Crucially, the occurrence of superconductivity in this family was not merely observed but predicted from electronic-structure calculations carried out in the same study: the calculated band structures exhibit van Hove singularities at the L point, producing the DOS maximum invoked under the van Hove scenario to explain the stabilization of Cooper pairing in this family (Winterlik et al., 2009). This combination of a priori theoretical prediction and subsequent experimental confirmation makes the Pd2ZrAl/Pd2HfAl/Pd2ZrIn/Pd2HfIn group a useful benchmark subfamily for testing first-principles methodology against experiment in Heusler superconductors more broadly.

Motivation and Scope of This Review

While Pd2ZrIn was among the four compounds reported in the original 2009 discovery (Winterlik et al., 2009) it has, until recently, received comparatively little dedicated follow-up study relative to some of its Heusler-superconductor relatives. A 2026 muon spin relaxation and rotation (μSR) study specifically targeting Pd2ZrIn has substantially advanced the microscopic picture of its superconducting ground state (Yadav et al., 2026) but to the best of the present review's literature search, no dedicated first-principles study of its structural, elastic/mechanical, vibrational (phonon), or electron-phonon-coupling properties has yet been published, in contrast to several related Heusler superconductors for which such calculations exist (e.g., HfPd2Al (Wiendlocha et al., 2015) LiPd2Si and LiPd2Ge (Górnicka et al., 2024; Górnicka et al., 2020)ScAu2Al (Kuderowicz & Wiendlocha, 2023)MgPd2Sb (Winiarski et al., 2021)). This review therefore has two aims: first, to consolidate the presently available experimental and theoretical literature on Pd2ZrIn into a single account of its structural, electronic, and superconducting properties; and second, to identify the specific computational gap, the absence of a dedicated structural/mechanical/vibrational DFT and DFPT study that remains open for future work, and to outline the methodological framework by which such a study, analogous to those performed for isostructural

compounds such as Ni2ZrAl (Mahdjouba et al., 2024) could be carried out.

Crystal Structure and Synthesis

$L2_1$ Structure and Site Occupation

Like the majority of Heusler superconductors, Pd2ZrIn adopts the cubic L21 full-Heusler structure (space group Fm3̄m, No. 225) (Graf et al., 2011; Winterlik et al., 2009; Górnicka et al., 2024). In this structure, Pd atoms occupy the 8c Wyckoff site, forming a cubic cage, while the Zr and In atoms occupy the 4a and 4b sites respectively, together completing a CaF2-type Zr2In-equivalent framework interpenetrated by the Pd sublattice (Graf et al., 2011; Górnicka et al., 2024). This crystal chemistry places Pd2ZrIn structurally alongside the majority of reported Heusler superconductors, in which the electronic "backbone" responsible for the Fermi-level density of states derives from the overlapping d orbitals of the transition-metal cage (Pd) (Górnicka et al., 2024).

B2-Type Antisite Disorder

A distinguishing structural feature of Pd2ZrIn, established by Rietveld refinement of powder X-ray diffraction data in the 2026 μSR study, is a substantial degree of B2-type antisite disorder superimposed on the underlying L21 lattice: the best fit to the diffraction pattern required approximately 50% site-mixing between the Zr (Y) and In (Z) sublattices (Yadav et al., 2026). Such B2 disorder in which the early transition metal and the p-block element partially exchange sites while the Pd cage remains ordered is a recurring feature in Heusler superconductors more broadly, and is known in related compounds (e.g., Ni2NbAl and other Nb-based Heusler alloys) to broaden the density of states near the Fermi level, introduce additional charge-carrier scattering centres, and produce spatial inhomogeneity in the superconducting gap, generally acting to suppress Tc relative to the fully ordered phase (Yadav et al., 2026). The presence and magnitude of this disorder is therefore an essential, sample-dependent parameter for interpreting the superconducting properties of Pd2ZrIn as earlier discussed, and is a plausible contributor to the modest spread between the Tc value reported for this specific compound in the most recent study (Yadav et al., 2026) and the wider 2.4–3.8 K range originally reported for the four-compound Pd-Zr/Hf-Al/In family collectively (Winterlik et al., 2009).

Synthesis

Consistent with the great majority of intermetallic Heusler superconductors in this class, polycrystalline Pd2ZrIn and its siblings are prepared by conventional high-temperature solid-state routes, which are typically arc-melting of the constituent elements under an inert atmosphere, followed by annealing to homogenize the sample and control the degree of antisite disorder, as is standard practice across this compound family (Winterlik et al., 2009; Górnicka et al., 2024; Yadav et al., 2026).

Electronic Structure and the Van Hove Scenario

The theoretical case for superconductivity in Pd2ZrIn rests on first-principles electronic-structure calculations reported alongside its experimental discovery (Winterlik et al., 2009). These calculations show that the band structure of the Pd2ZrAl/Pd2HfAl/Pd2ZrIn/Pd2HfIn family exhibits saddle-point (van Hove) singularities located at the L point of the Brillouin zone (Winterlik et al., 2009). Because a two-dimensional-like saddle point produces a logarithmically divergent, or at minimum sharply peaked, contribution to the electronic density of states, a Fermi level positioned at or near such a singularity yields an enhanced N(EF) that favours Cooper pairing according to the van Hove scenario, allowing bulk superconductivity to emerge even where the underlying electron-phonon coupling is only moderate (Winterlik et al., 2009). This mechanism is consistent with the broader pattern observed across VEC = 25–29 Heusler superconductors, in which the states at the Fermi level typically derive from antibonding combinations of the transition-metal cage d orbitals with s/p states of the main-group constituent — an antibonding character that has itself been proposed as a general correlate of superconductivity onset across several unrelated intermetallic families (Górnicka et al., 2024).

It should be noted explicitly that the computational gap is narrower than an absence of all first-principles information. Winterlik et al. (2009) included Pd_2ZrIn within family-level electronic-structure calculations that established the van Hove scenario. In addition, Yadav et al. (2026) derived $\lambda_{e-ph} \approx 0.56$ from experimental thermodynamic parameters using the McMillan expression. What remains unavailable in the literature located for this review is a dedicated Pd_2ZrIn-specific, self-consistent DFT/DFPT calculation of the equilibrium structure, elastic tensor, phonon spectrum, Eliashberg function $\alpha^2F(\omega)$, and ab initio electron–phonon coupling constant λ, of the kind performed for the closely related compound HfPd2Al under pressure (Wiendlocha et al., 2015) or for other Heusler superconductors such as ScAu2Al (Kuderowicz & Wiendlocha, 2023) and LiPd2Si/LiPd2Ge (Górnicka et al., 2024; Górnicka et al., 2020), does not yet appear in the published literature. The van Hove picture summarized above therefore currently rests on the original 2009 electronic-structure calculation for the compound family as a whole (Winterlik et al., 2009) rather than on a Pd2ZrIn-specific first-principles study incorporating the antisite disorder discussed previously, this of course represents one of the clearest openings for future computational work.

Superconducting Properties of Pd_2ZrIn

Original Characterization (2009)

In the original discovery report, Pd_2ZrIn was characterized, together with Pd_2ZrAl, Pd2HfAl, and Pd2HfIn, by electrical resistivity and magnetic-susceptibility measurements, which established bulk superconductivity in all four compounds with transition temperatures in the range Tc ≈ 2.4–3.8 K, and type-II behaviour under an applied magnetic field (Winterlik et al., 2009). This original study did not report compound-by-compound superconducting parameters (e.g., individual Tc values, upper critical fields, or electron-phonon coupling constants) for Pd_2ZrIn in isolation, treating the four compounds primarily as a group unified by the shared van Hove-driven mechanism.

Recent μSR Characterization (2026)

A substantially more detailed picture of the superconducting ground state specific to Pd2ZrIn was established by Yadav et al. (2026), who combined electrical resistivity, magnetic susceptibility, and zero-field and transverse-field muon spin relaxation/rotation (μSR) measurements. Resistivity and susceptibility data confirmed bulk, type-II superconductivity with Tc ≈ 2.2 K (Yadav et al., 2026). Zero-field μSR measurements below Tc revealed no evidence of spontaneous internal magnetic fields, demonstrating that time-reversal symmetry is preserved in the superconducting state, i.e., the pairing state is not of the time-reversal-symmetry-breaking type occasionally reported in other unconventional or unusual superconductors (Yadav et al., 2026). Transverse-field μSR spectra showed the formation of a flux-line (vortex) lattice, as expected for a type-II superconductor, and the resulting temperature dependence of the superfluid density was found to be well described by a single, fully gapped, nodeless s-wave order parameter, with a zero-temperature gap magnitude $\Delta(0) \approx 0.33 \pm 0.01$ meV (Yadav et al., 2026). Positioning Pd2ZrIn on the Uemura plot (the empirical correlation between Tc and the effective Fermi temperature TF derived from the superfluid density) places the compound within the conventional, weakly coupled BCS superconducting regime, rather than in the unconventional regime occupied by many high-Tc and heavy-fermion superconductors (Yadav et al., 2026). Heat-capacity analysis further yielded a Debye temperature of approximately 221 K and an electron–phonon coupling estimate $\lambda_{e-ph} \approx 0.56$ from the McMillan formalism, supporting the weak-coupling interpretation (Yadav et al., 2026). Taken together, these results establish Pd2ZrIn as a weakly coupled, dirty-limit, type-II superconductor with a fully gapped, nodeless s-wave pairing state and preserved time-reversal symmetry (Yadav et al., 2026).

Role of Antisite Disorder

The characterization of Pd2ZrIn as a dirty-limit superconductor in (Yadav et al., 2026) is directly connected to the substantial B2-type Zr/In antisite disorder discussed above. The μSR study explicitly frames Pd2ZrIn as a platform for studying the interplay between structural disorder and superconducting pairing within the Heusler family (Yadav et al., 2026). The preservation of a conventional, fully gapped s-wave state despite this substantial disorder is itself a notable finding, since strong antisite disorder is capable in principle of broadening the Fermi-level DOS enough to suppress the van Hove-enhanced pairing discussed earlier, or to introduce gap inhomogeneity; that the observed order parameter remains simple (single-gap, nodeless, non-time-reversal-symmetry-breaking) suggests that the conventional phonon-mediated pairing mechanism in this compound is comparatively robust against the observed level of disorder (Yadav et al., 2026).

Comparison with Related Heusler Superconductors

Table I situates Pd_2ZrIn among its closest structural and chemical relatives, which the other three compounds from the original 2009 discovery, the isostructural stannide $ZrPd_2Sn$, and a small set of other Pd-cage and VEC-comparable Heusler superconductors for which more complete parameter sets have been published which has enabled us to illustrate both the shared systematics of this compound class and the specific respects in which Pd_2ZrIn remains less thoroughly parameterized than several of its relatives.

Table 1: Pd_2ZrIn in the context of related Heusler superconductors

Compound	Structure	Tc (K)	Type	Coupling / λ	Notable feature	Ref.
Pd_2ZrIn	$L2_1$, ~50% B2 Zr/In disorder	~2.2	II	Weak (dirty limit)	Fully gapped nodeless s-wave; TRS preserved (μSR)	(Winterlik et al., 2009; Yadav et al., 2026)
Pd_2ZrAl	$L2_1$	2.4–3.8*	II	van Hove-assisted	Co-discovered with Pd_2ZrIn; predicted then confirmed	(Winterlik et al., 2009)
Pd_2HfAl	$L2_1$	2.4–3.8*	II	λ from DFT (pressure study)	Pressure-dependent λ and Tc calculated ab initio	(Winterlik et al., 2009; Wiendlocha et al., 2015)

Pd_2HfIn	$L2_1$	2.4–3.8*	II	van Hove-assisted	Co-discovered with Pd_2ZrIn	(Winterlik et al., 2009)
$ZrPd_2Sn$	$L2_1$ → tetragonal CDW phase	~1.2	—	—	Structural/CDW instability precedes SC	(Su et al., 2022)
$LiPd_2Si$	$L2_1$, VEC=25	1.3	I	λ = 0.49	s-block (Li) cage filler; DFT + COHP analysis	(Górnicka et al., 2024)
$MgPd_2Sb$	$L2_1$, VEC=27	2.2	II	Strong e–ph coupling	"Magic" VEC=27 predicted then confirmed	(Winiarski et al., 2021)
$ScAu_2Al$	$L2_1$	5.12	—	λ = 1.25	Highest reported Heusler Tc; SOC removes VHS	(Kuderowicz & Wiendlocha, 2023)

*Range reported for the four-compound family collectively in the original 2009 study, not resolved per-compound at that time (Winterlik et al., 2009).

Open Questions and Directions for First-Principles Study

Absence of a Dedicated Structural/Mechanical/ Vibrational DFT Study

As clarified earlier, previous work provides family-level electronic-structure calculations and experimental estimates of superconducting coupling parameters, but as of the literature search updated in June 2026, the literature located for this review does not contain a dedicated, comprehensive Pd_2ZrIn-specific DFT/DFPT characterization of its structural equilibrium parameters (optimized lattice constant, bulk modulus and its pressure derivative), elastic/mechanical properties (single-crystal and polycrystalline elastic constants, Young's and shear moduli, Poisson's ratio, Pugh's and Cauchy ductility/brittleness criteria, elastic anisotropy), or vibrational properties (phonon dispersion and density of states via density-functional perturbation theory, confirmation of dynamical stability, Debye temperature). This is a genuine gap relative to several closely related Heusler superconductors, for which such calculations have been published, for example, the pressure-dependent electronic, phonon, and electron-phonon-coupling study of the sibling compound $HfPd_2Al$ (Wiendlocha et al., 2015) and the DFT/DFPT study of structural, mechanical, electronic, vibrational, and superconducting properties recently reported for the isostructural Ni-cage analogues Ni_2ZrAl and Ni_2ZrGa (Mahdjouba et al., 2024). A directly analogous DFT + DFPT study of Pd_2ZrIn, following the same methodological template (norm-conserving or PAW pseudopotentials, a GGA-PBE exchange-correlation functional, structural relaxation, elastic-tensor calculation, and phonon-dispersion/DOS calculation via DFPT, followed by McMillan–Allen–Dynes estimation of Tc from the computed λ and Debye temperature) would both test the theoretical framework against the detailed experimental Tc, gap magnitude, and coupling regime already established by μSR (Yadav et al., 2026) and would supply the mechanical and vibrational property set presently missing from the literature.

Modelling the Effect of Antisite Disorder

A second, non-trivial open question is how best to incorporate the experimentally established ~50% B2-type Zr/In antisite disorder (Yadav et al., 2026) into a first-principles treatment of Pd2ZrIn, since standard DFT/DFPT calculations are most naturally performed on the fully ordered L21 structure. Approaches used elsewhere in the disordered-Heusler literature such as special quasirandom structures, supercell partial-occupancy models, or coherent-potential-approximation-based methods which could in principle be applied to determine whether the disorder-broadened DOS proposed qualitatively in (Yadav et al., 2026) is borne out quantitatively, and whether it is compatible with the robust, single-gap s-wave pairing observed experimentally.

Reconciling the Reported Tc Values

As noted in Table 1, a modest but unresolved discrepancy exists between the Tc ≈ 2.2 K reported for Pd2ZrIn specifically in the 2026 μSR study (Yadav et al., 2026) and the broader Tc ≈ 2.4–3.8 K range reported for the four-compound Pd–Zr/Hf–Al/In family collectively in 2009 (Winterlik et al., 2009). Because the original study did not isolate a compound-specific Tc for Pd2ZrIn, it is not possible from the published record alone to determine whether this reflects genuine sample-to-sample variation (e.g., differing degrees of antisite disorder between the two studies' samples, consistent with the disorder-sensitivity discussed earlier) or simply reflects that the 2009 range was dominated by the other three, higher-Tc members of the family. Resolving this would benefit from either a systematic disorder-controlled synthesis series or a first-principles study of how Tc depends on the degree of B2 disorder in this compound.

CONCLUSION

Pd2ZrIn is a well-established member of the Pd-based Heusler superconductor family, first predicted and confirmed as a type-II superconductor in 2009 and subsequently characterized in considerable microscopic detail by muon spin relaxation and rotation measurements, which establish bulk superconductivity at Tc ≈ 2.2 K with a fully gapped, nodeless s-wave order parameter, preserved time-reversal symmetry, and a weakly coupled, dirty-limit character reflecting substantial B2-type Zr/In antisite disorder. Its electronic structure is understood, at the level of the compound family as a whole, within the van Hove scenario, wherein saddle-point singularities at the Brillouin-zone L point enhance the Fermi-level density of states and favour phonon-mediated Cooper pairing. Despite this level of characterization, an important computational opportunity remains. The literature located for this review does not provide a dedicated, comprehensive Pd_2ZrIn-specific DFT/DFPT study that unifies structural optimization, elastic/mechanical properties, phonon dispersion, $\alpha^2F(\omega)$, and ab initio electron–phonon coupling, of the kind available for several related Heusler superconductors (Wiendlocha et al., 2015; Kuderowicz & Wiendlocha, 2023; Mahdjouba et al., 2024)leaving its elastic constants, phonon spectrum, dynamical stability, and computed electron-phonon coupling constant as clearly defined, tractable targets for future DFT/DFPT investigation.

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