

Supporting Information for

Synthetically Tuned Structural Variations in $\text{CePd}_x\text{Ge}_{2-x}$ ($x = 0.21, 0.32, 0.69$) towards Diverse Physical Properties

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Table S1. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) at 293(2) K with estimated standard deviations in parentheses.

Label	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
CePd_{0.32}Ge_{1.68}						
Ce	14(2)	14(2)	14(2)	7(1)	0	0
M	14(2)	14(2)	24(2)	7(1)	0	0
CePd_{0.21}Ge_{1.79}						
Ce	13(1)	13(1)	14(1)	0	0	0
M	29(1)	22(1)	23(1)	0	0	0
CePd_{0.69}Ge_{1.31}						
Ce1	12(2)	12(2)	6(4)	6(2)	0	0
Ce2	10(2)	10(2)	4(2)	5(1)	0	0
M1	12(3)	12(3)	14(4)	6(2)	0	0
M2	9(2)	9(2)	11(3)	5(1)	0	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$.

Table S2. Selected Bond lengths [$\text{\AA}$] at 293(2) K with estimated standard deviations in parentheses.

Label	Distances		
CePd_{0.32}Ge_{1.68}			
Ce-M	3.25148(13)	M-M	2.46026(11)
CePd_{0.21}Ge_{1.79}			
Ce-M	3.2240(8)	M1-M1	2.4223(12)
CePd_{0.69}Ge_{1.31}			
Ce1-M1	3.232(3)	M2-M2	2.4902(3)
Ce2-M2	3.231(3)		

Symmetry transformations used to generate equivalent atoms: ¹ x-1,y,-z (2) -x+1,-y,z (3) -x,-y-1,-z (4) x,y+1,z ¹ x,y,-z (6) -x,-y,z (7) -x+1,-y,-z+1 (8) -x,-y,-z+1 (9) -x,-y-1,-z+1 ¹ x-1,y,z (11) -x+1,-y-1,-z+1 (12) x,y-1,z (13) x+1,y,z (14) -x,-y-1,z (15) -x+1,-y-1,z

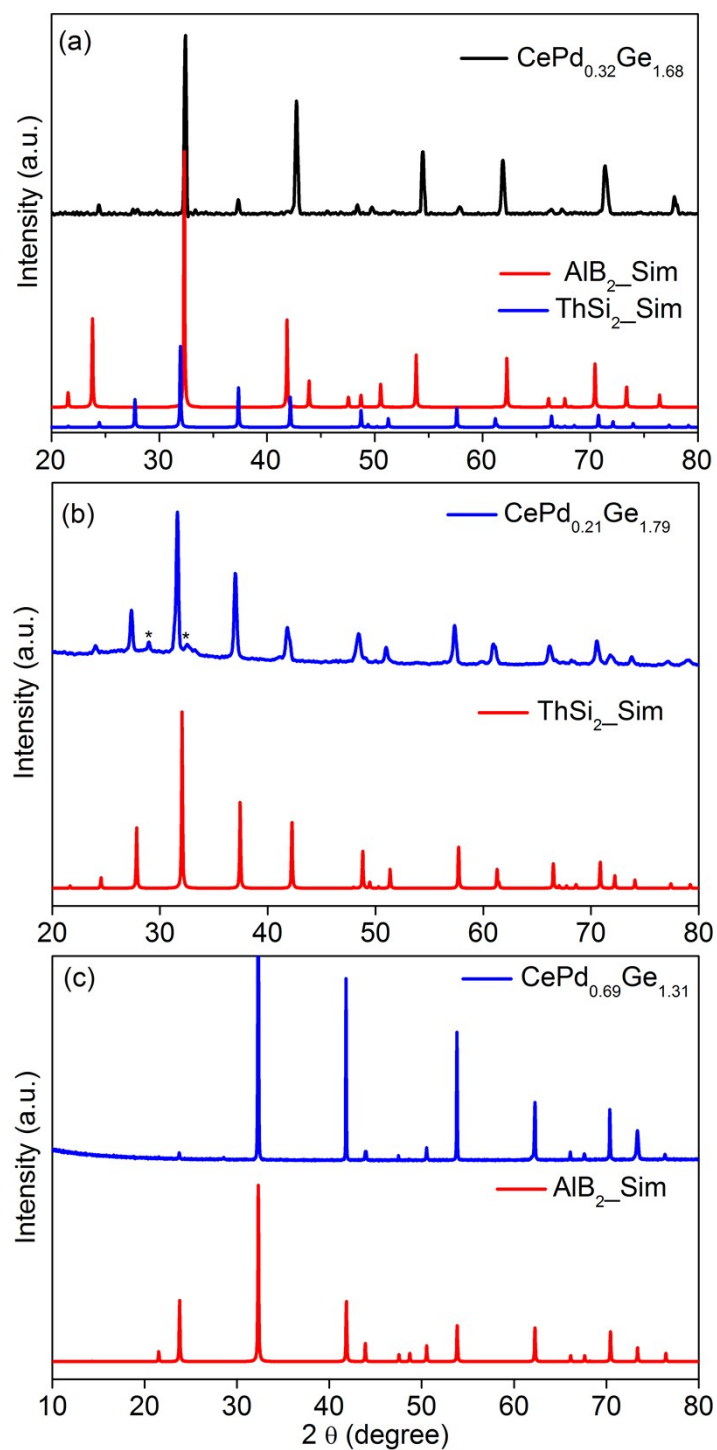


Figure S1. Comparison of experimental PXRD patterns of (a) CePd_{0.32}Ge_{1.68}, (b) CePd_{0.21}Ge_{1.79} and (c) CePd_{0.69}Ge_{1.31} with simulated structures crystallize in the AlB₂ and α -ThSi₂ structure types obtained from the single crystal structure refinement.

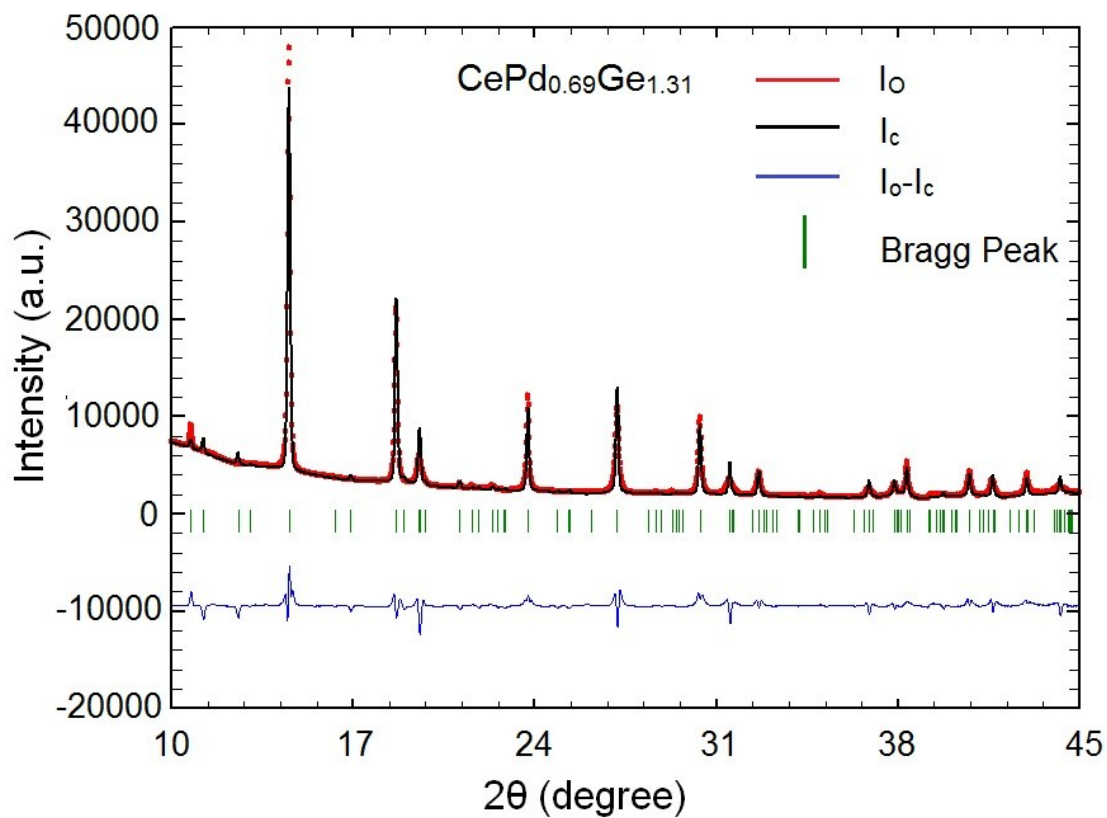


Figure S2. Rietveld refinement of synchrotron PXRD data collected on $\text{CePd}_{0.69}\text{Ge}_{1.31}$ at 0.7 Å wavelength using the simulated PXRD data obtained from the SCXRD refinement.