

Electronic Supplementary Information

New Phases of 3d-Transition Metal-Cerium Binary Compounds: An Extensive Structural Search

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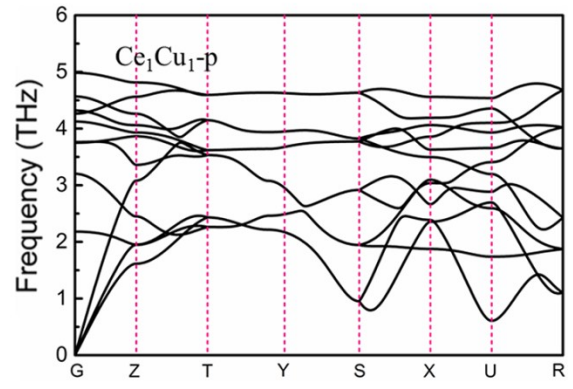
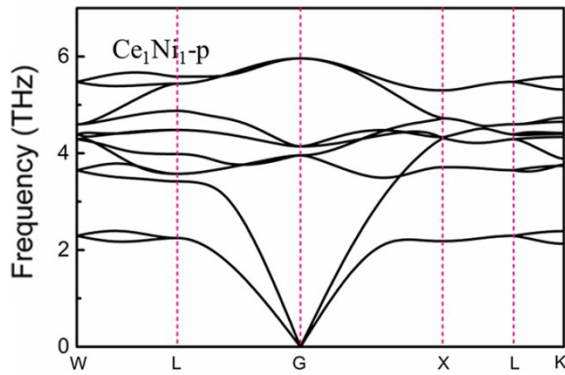
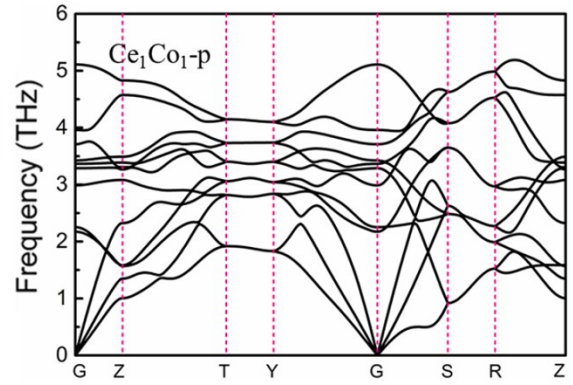
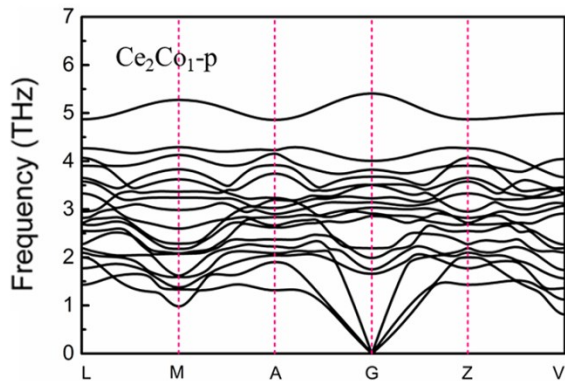
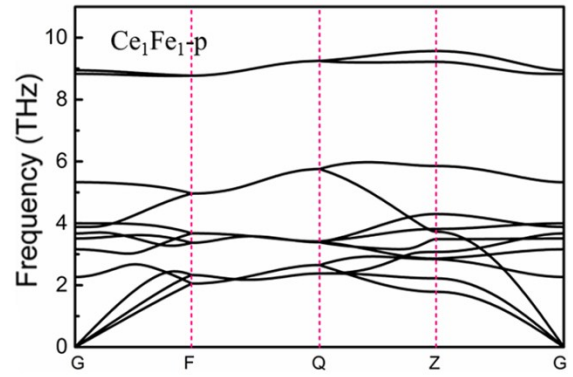
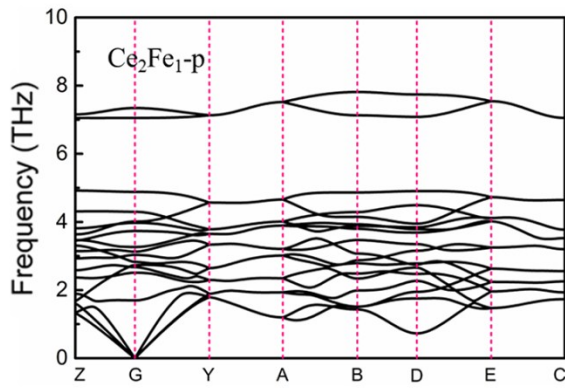
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(a)



(b)

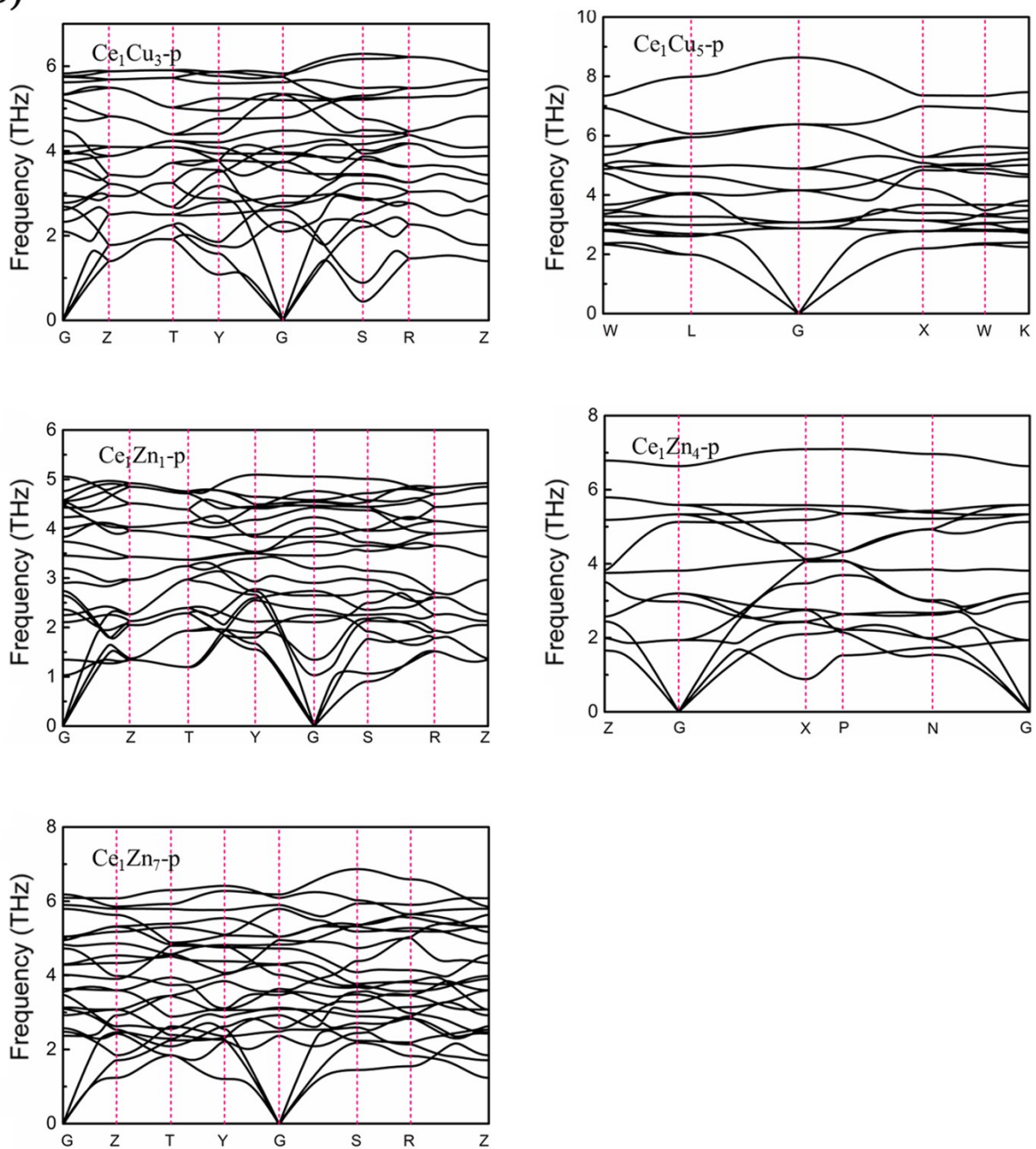


Fig. S1. The phonon spectra of all the predicted phases.

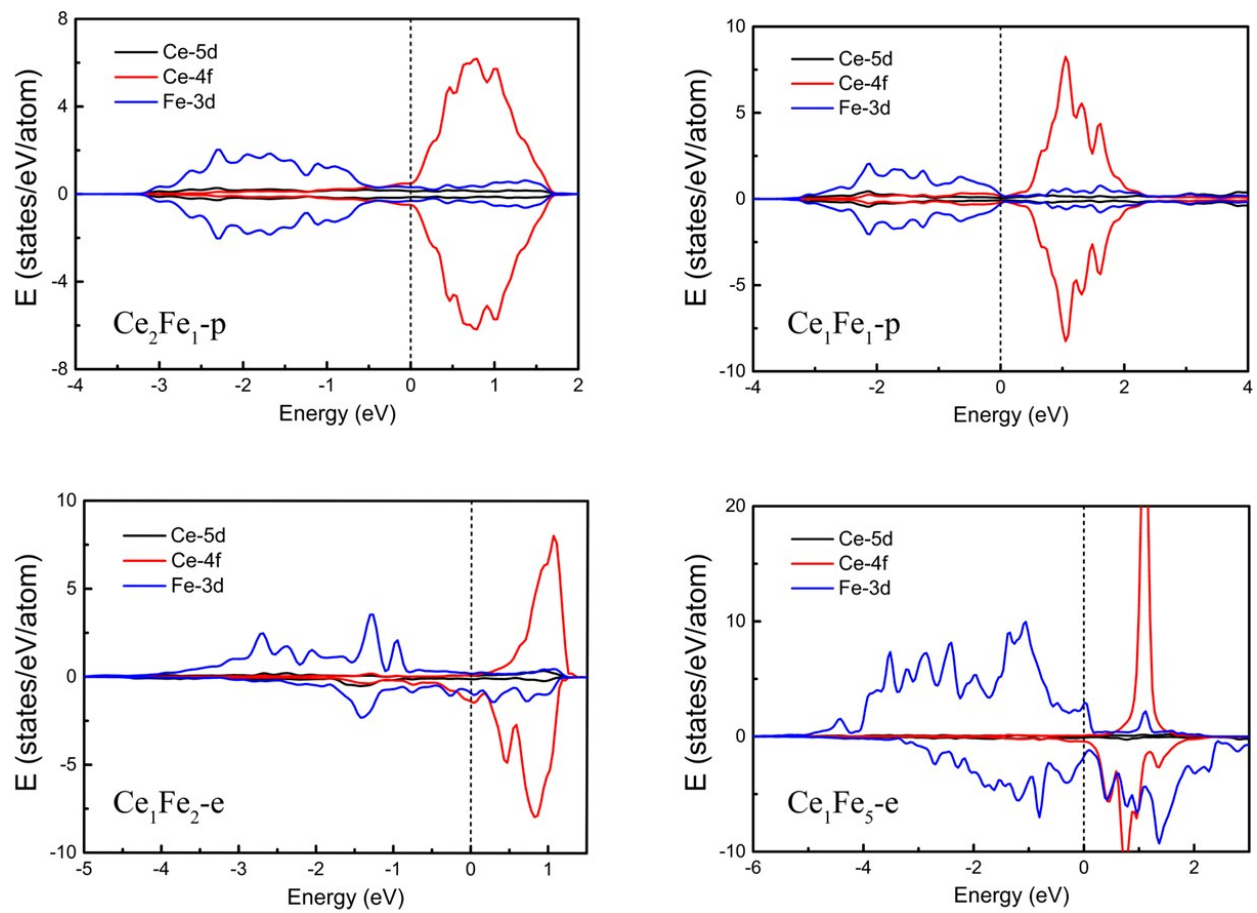


Fig. S2. The PDOS of the Ce-Fe system.

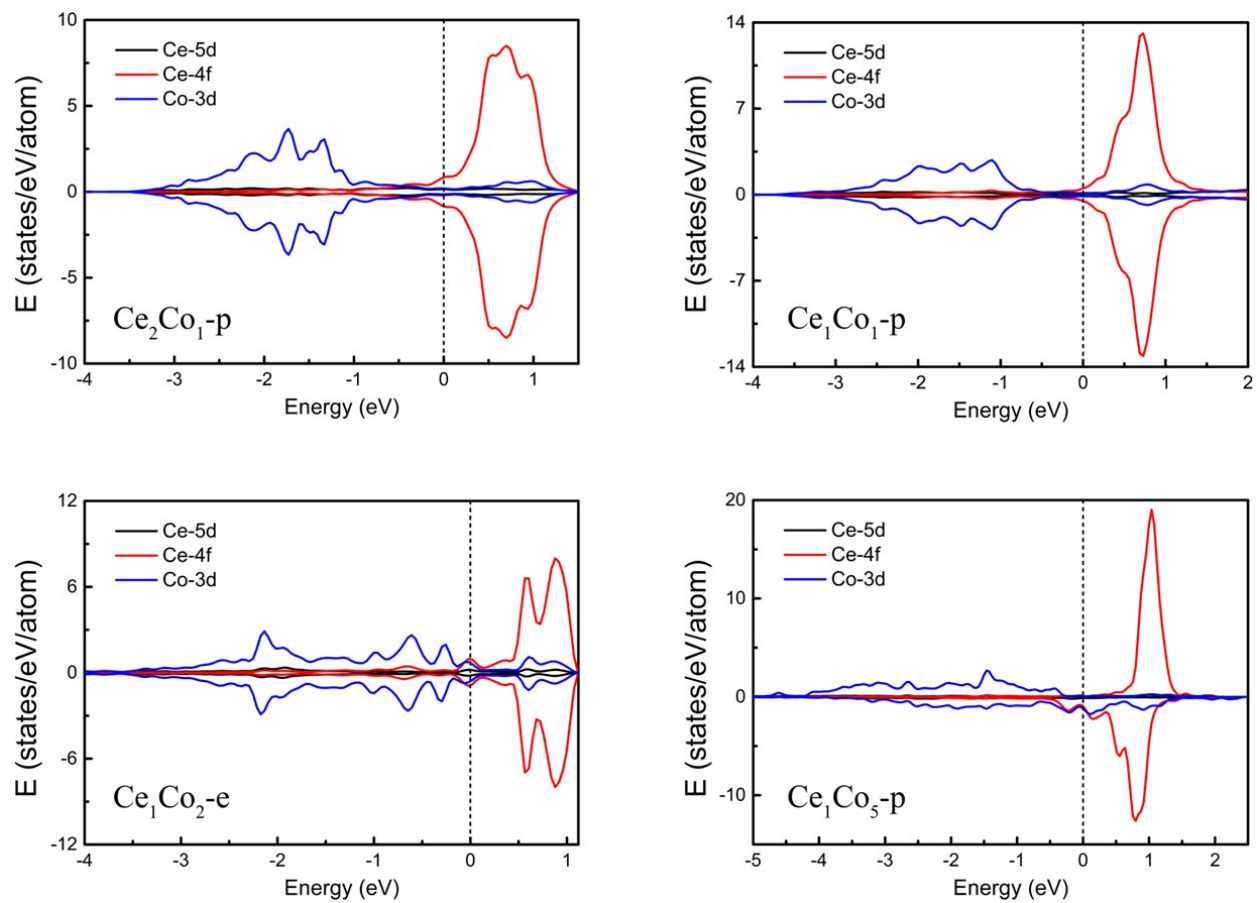


Fig. S3. The PDOS of the Ce-Co system.

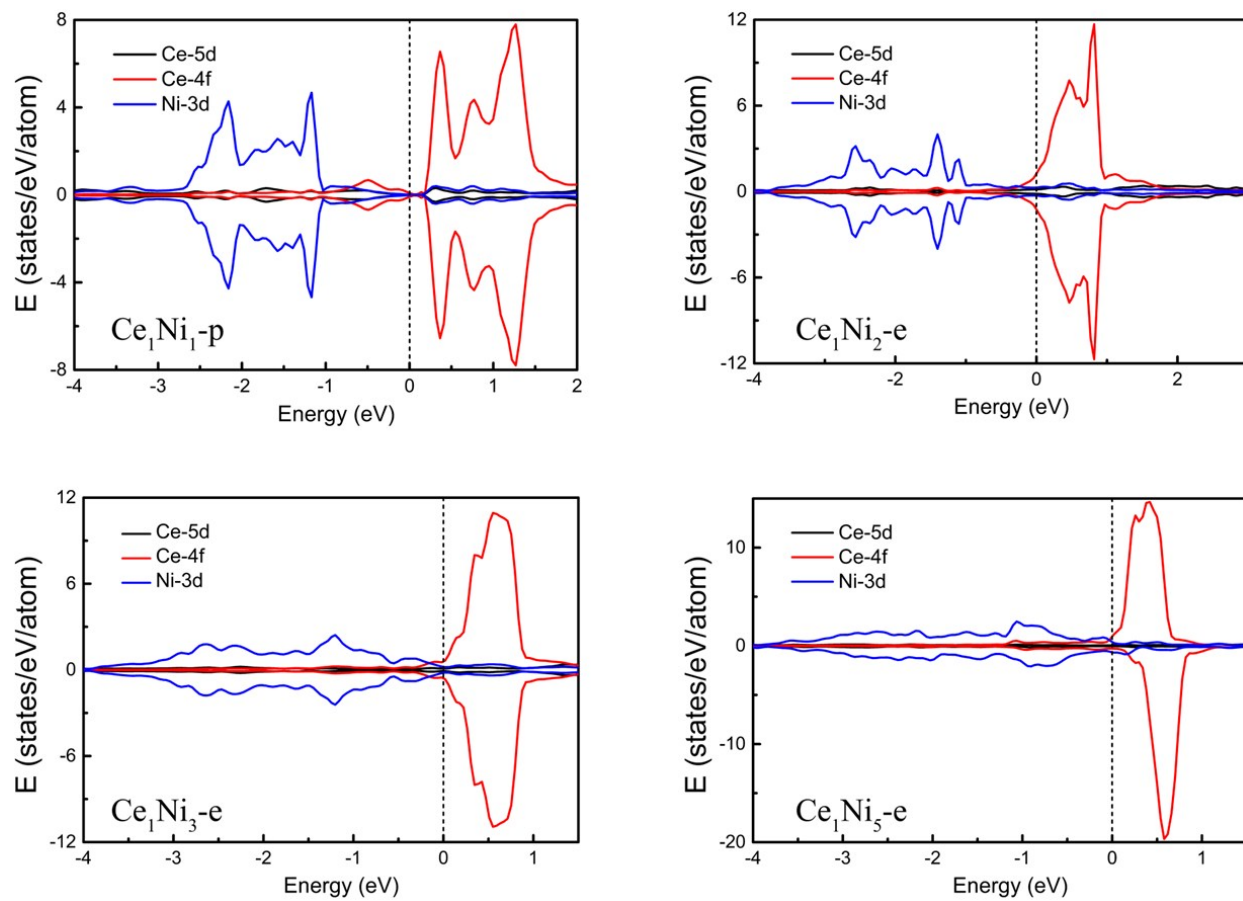


Fig. S4. The PDOS of the Ce-Ni system.

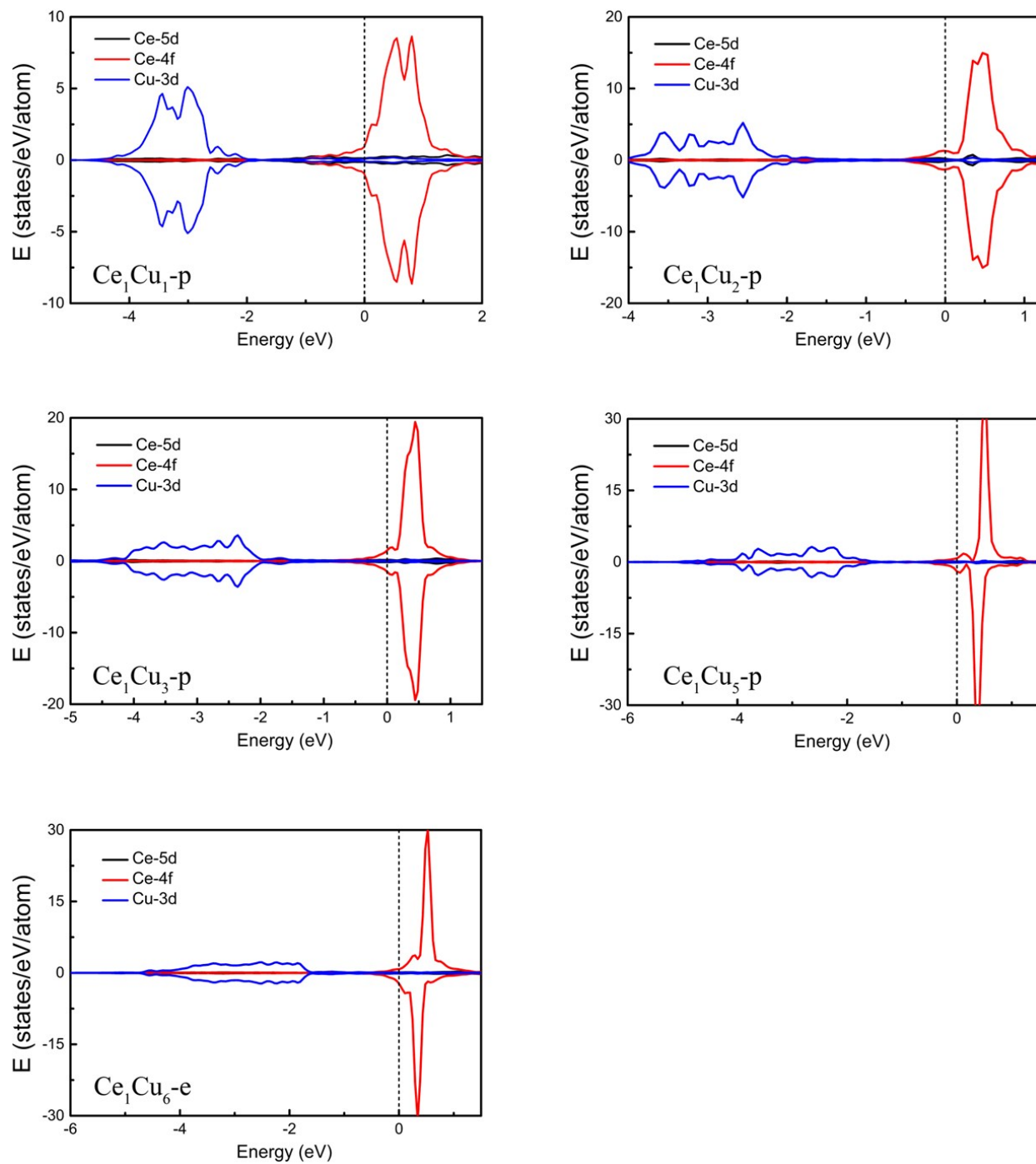


Fig. S5. The PDOS of the Ce-Cu system.

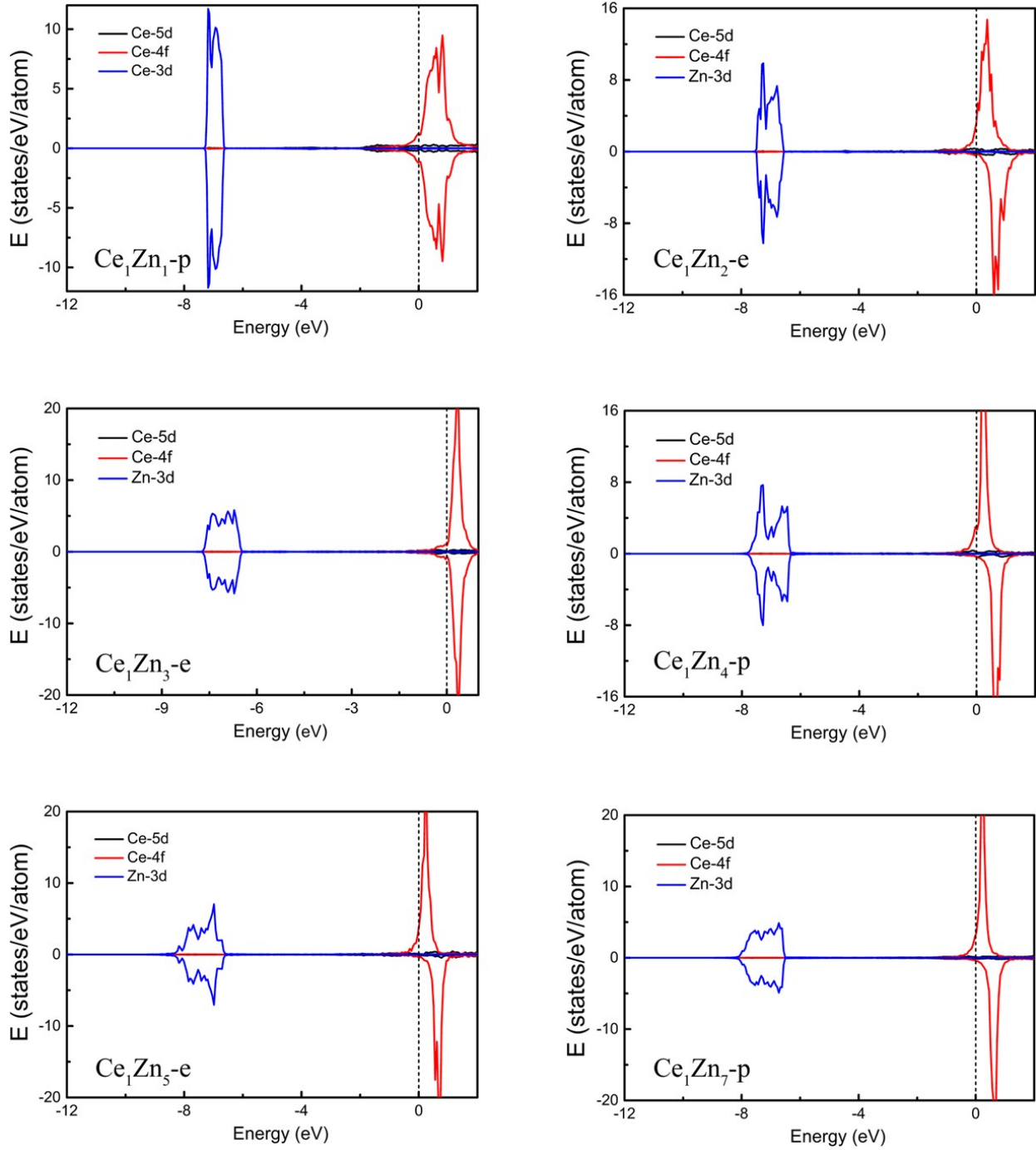


Fig. S6. The PDOS of the Ce-Zn system.

Table S1. The elastic constants C_{ij} (GPa) for the Ce-TM (TM=Fe, Co, Ni, Cu, Zn) systems.

Phases	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}
Ce ₂ Fe ₁ -p	106	81	65	38	14	30	52	46	26
Ce ₁ Fe ₁ -p	83	100	168	41	10	33	49	53	72
Ce ₁ Fe ₂ -e	119	119	119	18	18	18	83	83	83
Ce ₁ Fe ₅ -e	178	178	167	64	64	50	78	65	65
Ce ₂ Co ₁ -p	99	89	114	23	34	26	25	42	41
Ce ₁ Co ₁ -p	150	124	85	22	13	9	84	46	48
Ce ₁ Co ₂ -e	191	191	191	27	27	27	120	120	120
Ce ₁ Co ₅ -e	206	206	278	49	49	36	133	112	112
	192	192	259	45	45	45	131	108	108
Ce ₁ Ni ₁ -p	185	185	185	79	79	79	96	96	96
Ce ₁ Ni ₂ -e	187	187	192	42	42	46	95	91	91
Ce ₁ Ni ₃ -e	169	169	184	43	43	50	69	47	47
Ce ₁ Ni ₅ -e	221	221	269	69	69	56	109	87	87
Ce ₁ Cu ₁ -p	138	101	62	42	51	45	70	17	42
Ce ₁ Cu ₂ -e	151	151	56	30	30	34	84	62	62
Ce ₁ Cu ₃ -p	107	179	60	30	66	29	57	45	40
Ce ₁ Cu ₅ -p	118	118	118	50	50	50	46	46	46
Ce ₁ Cu ₆ -e	148	119	178	4	52	9	82	53	73
Ce ₁ Zn ₁ -p	111	80	99	48	41	20	22	33	29
Ce ₁ Zn ₂ -e	104	109	115	36	33	21	43	43	44
Ce ₁ Zn ₃ -e	101	101	98	25	25	22	58	62	61
Ce ₁ Zn ₄ -p	113	110	106	33	30	31	49	47	49
Ce ₁ Zn ₅ -e	121	121	138	56	56	31	60	51	51
Ce ₁ Zn ₇ -p	109	143	117	39	41	51	36	54	34