Anhang zur Dissertation:

DFT-Vorhersage der Kristallstruktur und Eigenschaften intermetallischer Actinoidverbindungen

Die Beispiele UCo und UIr

Dissertation

zur Erlangung des akademischen Grades
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A.1.1 Details zu den verwendeten Basissätzen

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Element	PAW-Basis	Valenz	COHP-Basis
Ti[1]	Ti.pbe-spn-kjpaw_psl.1.0.0.UPF	$4s^2 3s^2 3p^6 3d^2$	4s 3s 3p 3d
Zr[1]	Zr.pbe-spn-kjpaw_psl.1.0.0.UPF	$5s^2 4s^2 4p^6 4d^2$	5s 4s 4p 4d
Nd[2]	Nd.GGA-PBE-paw-v1.0.UPF	$6s^2 5s^2 5p^6 5d^1 4f^3$	6s 5s 5p 5d 4f
Th†	Th.pbe-spn-kjpaw_MS.UPF	$7s^2 6s^2 6p^6 6d^{1.9} 5f^{0.1}$	7s 6s 6p 6d 5f
Pa†	Pa.pbe-spn-kjpaw_MS.UPF	$7s^2 6s^2 6p^6 6d^1 5f^2$	7s 6s 6p 6d 5f
U†	U.pbe-spn-kjpaw_MS.UPF	$7s^2 6s^2 6p^6 6d^1 5f^3$	7s 6s 6p 6d 5f
Np†	Np.pbe-spn-kjpaw_MS.UPF	$7s^2 6s^2 6p^6 6d^1 5f^4$	7s 6s 6p 6d 5f
Pu†	Pu.pbe-spn-kjpaw_MS.UPF	$7s^2 6s^2 6p^6 6d^0 5f^6$	7s 6s 6p 6d 5f
Co[1]	Co.pbe-n-kjpaw_psl.0.2.3.UPF	$4s^2 3d^7$	4s 3d
Rh[1]	Rh.pbe-spn-kjpaw_psl.1.0.0.UPF	$5s^2 4s^2 4p^6 4d^7$	5s 4s 4p 4d
Ir[1]	Ir.pbe-n-kjpaw_psl.0.2.3.UPF	$6s^2 5d^7$	6s 5d
Pd[1]	Pd.pbe-n-kjpaw_psl.0.3.0.UPF	$5s^{0.5} 4d^{9.5}$	–
Pt[1]	Pt.pbe-n-kjpaw_psl.0.1.UPF	$5s^1 4d^9$	–
Bi[1]	Bi.pbe-dn-kjpaw_psl.0.2.2.UPF	$6s^2 6p^3 5d^1 0$	–

† Daten aus dieser Doktorarbeit.

Tabelle A.1.2: Verwendete MT-Radien und Valenzelektronenkonfiguration für die verwendeten APW+2LO-Basisfunktionen.

Element	MT-Radius / a.u.	Valenz
Co	2.4	$4s^2 3p^6 3d^7$
Rh	2.6	$5s^1 4s^2 4p^6 5d^8$
Ir	2.6	$6s^2 5s^2 5p^6 5d^7$
U	3.0	$7s^2 6s^2 6p^6 6d^1 5f^3$

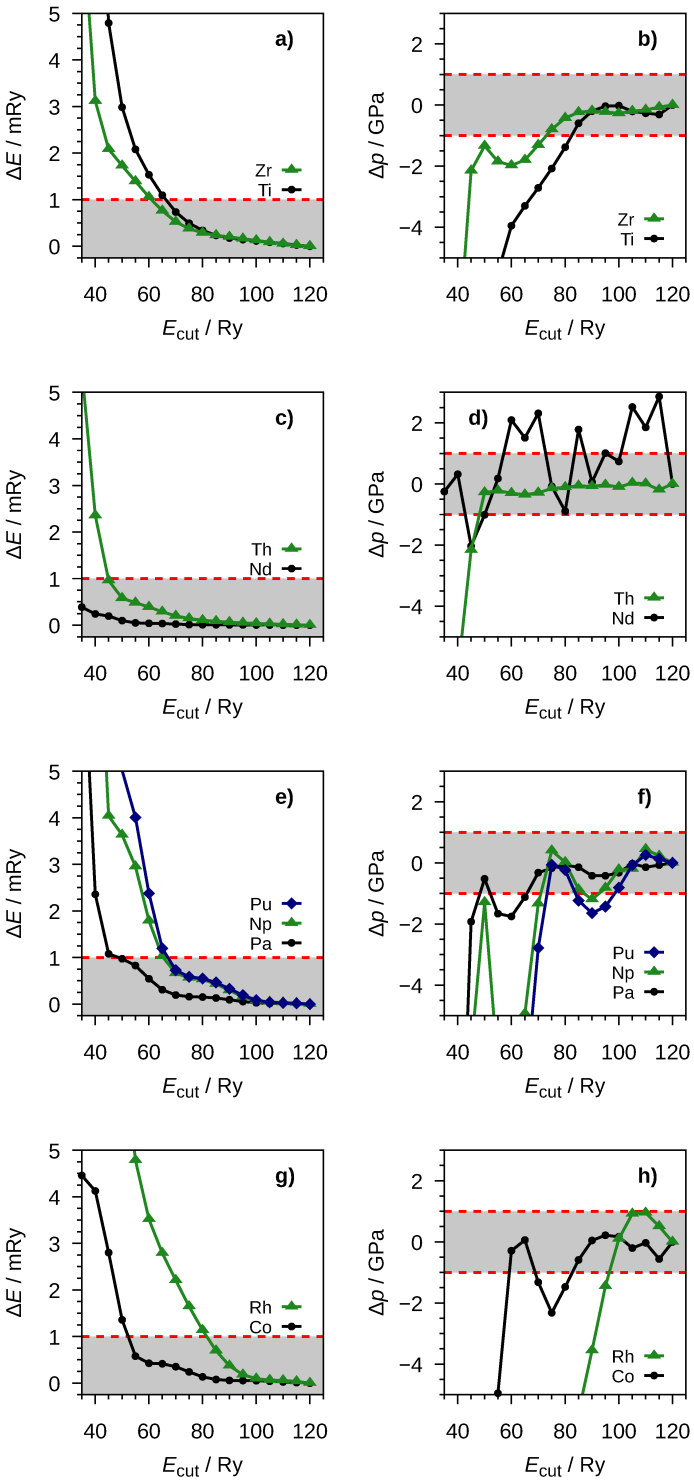

Abbildung A.1.1: PAW-Basissatzkonvergenz in Bezug auf relative Gesamtenergie ΔE und relativen Druck Δp. **(a)** ΔE von Ti- und Zr-PAW-Basis, **(b)** Δp von Ti- und Zr-PAW-Basis, **(c)** ΔE von Nd- und Th-PAW-Basis, **(d)** Δp von Nd- und Th-PAW-Basis, **(e)** ΔE von Pa-, Np- und Pu-PAW-Basis, **(f)** Δp von Pa-, Np- und Pu-PAW-Basis, **(g)** ΔE von Co- und Rh-PAW-Basis, **(h)** Δp von Co- und Rh-PAW-Basis. PBE-Rechnungen in bcc-Struktur ohne Spinpolarisation und skalar-relativistischer PAW-Basis.

A.1.2 Input-Dateien für modifizierte Elk-Basissätze

APW+2LO-Basis für Ir-Atome

```
'Ir'
'iridium'
-77.0000
350390.1559
0.227921E-06    2.6000   41.0330   700
22
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    F
5   1   1   2.00000    F
5   1   2   4.00000    F
5   2   2   4.00000    F
5   2   3   3.00000    F
6   0   1   2.00000    F
1
0.1500   0  F
0
5
0   2
0.1500   0  F
0.1500   1  F
1   2
0.1500   0  F
0.1500   1  F
2   2
0.1500   0  F
0.1500   1  F
0   3
0.1500   0  F
0.1500   1  F
-2.9000   0  T
1   3
0.1500   0  F
0.1500   1  F
-1.8716   0  T
```

APW+2LO-Basis für U-Atome

```
'U'
'uranium'
-92.0000
433900.1591
0.208514E-06    3.000   55.1377   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    T
5   2   3   6.00000    T
5   3   3   3.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2  1.000000    F
7   0   1   2.00000    F
1
0.1500   0  F
0
6
0   2
0.1500   0  F
0.1500   1  F
1   2
0.1500   0  F
0.1500   1  F
2   2
0.1500   0  F
0.1500   1  F
3   2
0.1500   0  F
0.1500   1  F
0   3
0.1500   0  F
0.1500   1  F
-1.7461   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.7688   0  T
```

A.1.3 Startparameter für Strukturoptimierungen in Kapitel 6.4: DFT-Rechnungen ausgewählter Strukturtypen

Tabelle A.1.3: Startparameter für die Strukturtypen der Strukturoptimierungen der MN-Verbindungen mit *Quantum ESPRESSO*. Der Parameter `Celldm(1)` wurde aus den Atomvolumina abgeschätzt. Die M- und N-Atome besetzten jeweils nur eine Punktlage beschrieben über die relativen Koordinaten x, y und z.

Parameter	Strukturtyp					
	CrB	CsCl	NaTl	UCo	TiNi	FeB
`Celldm(2)`	2.8	1.0	1.0	1.0	1.0	0.65
`Celldm(3)`	1.1	1.0	1.0	1.0	0.71	0.8
`Celldm(5)`	0.0	0.0	0.0	0.0	−0.1	0.0
$x(M)$	0.00	0.0	0.0	0.03	0.26	0.125
$y(M)$	0.85	0.0	0.0	0.03	0.25	0.25
$z(M)$	0.25	0.0	0.0	0.03	0.01	0.625
$x(N)$	0.00	0.5	0.5	0.29	0.74	0.0
$y(N)$	0.60	0.5	0.5	0.29	0.25	0.25
$z(N)$	0.25	0.5	0.5	0.29	0.01	0.125

A.2 Anhang Kapitel 4: Technische Details zu den experimentellen Untersuchungen

A.2.1 Syntheseparameter

Tabelle A.2.1: Syntheseparameter der hergestellten Verbindungen. Synthese im Lichtbogen (LB), Anlassen in Ta-Ampullen, Mörsern und Pressen (MP), Stress-Reduktion (SR) der pulverförmigen Proben in Ta-Ampullen.

Probe	Zusammensetzung	LB	Anlassen	SR
BC19	$UCo_{0.2}Rh_{0.8}$	√	6 d bei 720 °C	X
BC30	$UCo_{0.1}Rh_{0.9}$			
BC31	$UCo_{0.3}Rh_{0.7}$	√	33 d bei 680 °C	X
BC32	$UCo_{0.4}Rh_{0.6}$			
BC45	$UCo_{0.15}Rh_{0.85}$			
BC46	$UCo_{0.5}Rh_{0.5}$	√	48 d bei 680 °C	X
BC47	$UCo_{0.6}Rh_{0.4}$			
MSa38	UCo	√	10 d bei 695 °C, MP + 7 d bei 695 °C	X
MSa42temp	UCo	√	30 d bei 700 °C	1d bei 600 °C
BC44temp	UCo	√	6 d bei 795 °C	1d bei 600 °C
BC09	UIr	√	X	12h bei 600 °C, 7d bei 200 °C
MSa78	UIr	√	Einkristallzucht (s. Text)	

A.2.2 Details zu den Rietveld-Verfeinerungen

Tabelle A.2.2: Technische Daten zur Messung und Rietveld-Verfeinerung von UCo (Probe MSa42_temp).

Messbedingungen			
Probe	MSa42_temp		
Diffraktometer, Generator Einstellungen	Stoe STADI MP; 40 kV, 40 mA		
Strahlung, Sekundärmonochromator	Cu $K_{\alpha 1}$, Ge(111)		
Geometrie	Transmission		
Probendrehung	ja		
Messbereich, Schrittweite (2θ) / °	20-106, 0.015		
Messzeit pro Schritt / s	25		
Temperatur T / K	298		
Globale Parameter			
Software	JANA2006		
Anzahl benutzter Phasen	3		
Anzahl Variablen	26		
Nullpunktsverschiebung	1.4(2)		
Typ der Profilfunktion	Pseudo-Voigt		
Profil-Basisweite	10*(FWHM)		
Asymmetrie	Finger *et al.*		
Untergrundbehandlung	Polynomfunktion 8. Grades		
Strukturdaten			
Farbe des Pulvers	metallisch grau		
Formel	$U_{1.04}Co_{0.96}$	UCo_2	UO_2
Molare Masse M / g mol^{-1}	297.0	355.9	270.0
Raumgruppe (Nr.)	$I2_13$ (Nr. 199)	$Fd\bar{3}m$ (Nr. 227)	$Fm\bar{3}m$ (Nr. 225)
Pearson-Symbol	$cI16$	$cF24$	$cF12$
a / Å	6.3586(2)	7.0118(5)	5.4718(9)
V / Å^3	257.120(9)	344.740(6)	163.829(4)
Z	8	8	4
Röntgenographische Dichte D_x / g cm^{-3}	15.34	14.50	10.95
Massenanteil ω / %	74(2)	18(2)	8(1)
$\Delta\rho_{\min}, \rho_{\max}$/ e · Å^{-3}	−3.25, 3.4	–	–
R_{Bragg}/ %	7.2	14	14
globale Residualwerte			
R_{Profil} / %	6.4		
R_{wProfil} / %	8.2		
GOF	1.1		

Tabelle A.2.3: Technische Daten zur Messung und Rietveld-Verfeinerung von $UCo_{0.3}Rh_{0.7}$ (Probe BC31).

Messbedingungen	
Probe	BC31
Diffraktometer, Generator Einstellungen	Stoe STADI MP; 40 kV, 40 mA
Strahlung, Sekundärmonochromator	Cu $K_{\alpha 1}$, Ge(111)
Geometrie	Transmission
Probendrehung	ja
Messbereich, Schrittweite (2θ) / °	10-85, 0.015
Messzeit pro Schritt / s	20
Temperatur T / K	298
Globale Parameter	
Software	Jana2006
Anzahl benutzter Phasen	1
Anzahl Variablen	17
Typ der Profilfunktion	Lorentz
Profil-Basisweite	10*(FWHM)
Untergrundbehandlung	Polynomfunktion 10. Grades
Strukturdaten	
Farbe des Pulvers	metallisch grau
Formel	$UCo_{0.20(2)}Rh_{0.80}$
Molare Masse M / g mol^{-1}	332.1
Raumgruppe (Nr.)	$Fd\bar{3}m$ (Nr. 227)
Pearson-Symbol	$cF16$
a / Å	6.4477(2)
V / Å^3	268.050(5)
Z	8
Röntgenographische Dichte D_x / g cm^{-3}	16(3)
$\Delta\rho_{\min}, \rho_{\max}$ / e · Å^{-3}	−0.93, 0.77
R_{Bragg} / %	1.7
globale Residualwerte	
R_{Profil} / %	5.8
R_{wProfil} / %	7.5
GOF	1.0

Tabelle A.2.4: Technische Daten zur Messung und Rietveld-Verfeinerung von UIr (Probe BC09).

Messbedingungen	
Probe	BC09
Diffraktometer	P02.1, PETRA III (DESY, Hamburg)
λ / Å (Synchrotron)	0.20709
Geometrie	Debye-Scherrer
Probendrehung	ja
Messbereich, Schrittweite (2θ) / °	1.13-13.12, 0.003
Temperatur T / K	298
Globale Parameter	
Software	Jana2006
Anzahl benutzter Phasen	1
Anzahl Variablen	44
Anzahl an Restrains	0
Anzahl an Constrains	8
Typ der Profilfunktion	Pseudo-Voigt
Profil-Basisweite	12*(FWHM)
Anisotrope Partikelverbreiterung	Kugelflächenfunktionen 4. Grades
Anisotrope Spannungsverbreiterung	Tensormethode nach Stephens
Untergrundbehandlung	Polynomfunktion 14. Grades
Strukturdaten	
Farbe des Pulvers	metallisch grau
Formel	UIr
Molare Masse M / g mol^{-1}	430.25
Raumgruppe (Nr.)	$P2_{/c}$ (Nr. 14)
Pearson-Symbol	$mP16$
a / Å	5.6119(6)
b / Å	10.5862(7)
c / Å	5.5908(7)
β / °	98.944(7)
V / 10^6 pm^3	328.10(6)
Z	8
Röntgenographische Dichte D_x / g cm^{-3}	17.42
$\Delta\rho_{\min}, \rho_{\max}$ / e · Å^{-3}	−1.71 / 1.75
R_{Bragg} / %	2.9
globale Residualwerte	
R_{Profil} / %	4.9
R_{wProfil} / %	5.8
GOF	3.7

A.2.3 Details zur Einkristallstrukturanalyse von UIr

Tabelle A.2.5: Technische Daten zur Einkristallstrukturanalyse von UIr (Probe MSa78). Die Zellparameter stammen aus der Rietveld-Verfeinerung, Tabelle A.2.4.

Probe	MSa78
Chemische Formel	UIr
Molmasse / g mol^{-1}	430.23
Raumgruppe	$P2_1/c$ (Nr. 14)
Pearson-Symbol	$mP16$
Z	8
a / Å	5.6119(6)
b / Å	10.5862(7)
c / Å	5.5908(7)
β / °	98.944(7)
V / Å^3	328.10(6)
Röntgenographische Dichte D_x / g cm^{-3}	17.42
Absorptionskoeffizient μ / mm^{-1}	178.9
Kristallabmessungen / μm^3	45 x 50 x 71
Kristallform	Keil
Diffraktometer	IPDS-2 (Stoe & Cie.)
Strahlung	Mo K$_\alpha$
T / K	293
Abstand Kristall-IP / mm	55
$\omega_{min} - \omega_{max}$ / °	0-180, 60-130, 0-60
$\Delta\omega$ / °	1.2
ϕ / °	274, 160, 85
Belichtungszeit / min	30
Filter	nein
Anzahl gemessener Reflexe	13815
$2\theta_{min} - 2\theta_{max}$ / °	7.4 bis 70 (abgeschnitten bei 65°)
Miller-Index-Bereich, hkl	−8 bis +8, −16 bis +17, -8 bis +8
Datenreduktion	IPDS-Software, X-RED
Absorptionskorrektur	numerisch
T_{min} / T_{max}	0.0049 / 0.0485
R_{int}, R_σ	0.127, 0.057
Anzahl unabhängiger Reflexe	1212
Vollständigkeit des Datensatzes	99 %
Strukturverfeinerung	Methode der kleinsten Fehlerquadrate mit vollständiger Matrix (SHELXL-2006)
Anzahl Parameter	30
Anzahl an Restrains	0
Anzahl an Constrains	8
$R_1(F)$ ($I > 2\sigma(I)$)	0.044
$R_1(F)$ (alle Daten)	0.062
$wR_1(F^2)$ ($I > 2\sigma(I)$)	0.109
$wR_2(F^2)$ (alle Daten)	0.126
S (F^2) (alle Daten)	1.139
Zwillingsverhältnis	0.481(3)
$\Delta\rho_{min}, \rho_{max}$/ e · Å^{-3}	−6.83 / 6.77

A.3 Anhang zu Kapitel 6: Kristallstrukturvorhersage der binären Verbindungen UCo und UIr

A.3.1 Optimierte Strukturen der *MN*-Verbindungen mit dem GGA-PBE-Funktional

Tabelle A.3.1: Ergebnisse der PBE-Strukturoptimierungen der MN-Verbindungen im CsCl-, NaTl- und UCo-Typ. Gitterparameter, Lageparameter vom UCo-Typ (Punktlage 8a) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

N	M	CsCl-Typ		NaTl-Typ		UCo-Typ			
		a/Å	$\Delta H/\frac{\text{kJ}}{\text{mol}}$	a/Å	$\Delta H/\frac{\text{kJ}}{\text{mol}}$	a/Å	$x(M)$	$x(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	2.974	−36.1	5.903	−11.8	5.947	0.000	0.2500	−36.1
	Zr	3.177	−27.7	6.266	6.3	6.356	0.0000	0.250	−27.7
	Th	3.459	−7.0	6.762	27.0	6.898	0.008	0.285	−11.0
	Pa	3.308	−10.8	6.418	−21.9	6.501	0.026	0.293	−32.3
	U	3.241	8.7	6.234	−26.6	6.308	0.035	0.297	−26.4
	Np	3.275	22.0	6.075	−17.7	6.178	0.047	0.306	−4.7
	Pu	3.318	4.9	6.030	0.3	6.539	0.023	0.294	3.3
	Nd	3.399	−7.9	6.482	2.2	6.844	0.000	0.250	−9.0
Rh	Ti	3.109	−69.2	6.206	−41.5	6.219	0.000	0.250	−69.4
	Zr	3.293	−73.2	6.507	−42.1	6.584	0.000	0.250	−73.2
	Th	3.564	−67.2	6.940	−39.4	7.120	0.010	0.279	−68.2
	Pa	3.435	−53.9	6.664	−66.8	6.766	0.031	0.288	−67.8
	U	3.405	−29.4	6.515	−58.2	6.604	0.040	0.291	−46.5
	Np	3.406	−19.8	6.390	−37.3	6.544	0.048	0.296	−21.1
	Pu	3.424	−43.4	6.668	−32.5	6.845	0.000	0.250	−43.3
	Nd	3.490	−62.8	6.711	−42.0	6.954	0.001	0.252	−46.9
Ir	Ti	3.125	−75.0	6.244	−46.5	6.251	0.006	0.260	−75.8
	Zr	3.308	−77.8	6.534	−44.8	6.618	0.003	0.257	−77.9
	Th	3.579	−70.1	6.959	−36.1	7.157	0.008	0.275	−71.1
	Pa	3.461	−61.1	6.708	−67.8	6.814	0.031	0.287	−73.9
	U	3.427	−36.9	6.578	−58.2	6.657	0.040	0.290	−54.7
	Np	3.423	−25.6	6.535	−36.2	6.725	0.033	0.286	−24.4
	Pu	3.435	−45.0	6.677	−32.2	6.867	0.002	0.253	−45.0
	Nd	3.493	−60.8	6.750	−38.1	6.978	0.015	0.283	−60.8

Tabelle A.3.2: Ergebnisse der PBE-Strukturoptimierungen der MN-Verbindungen im CrB-Typ. Gitterparameter, y-Lageparameter (Punktlage 4c) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalarrelativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	$y(M)$	$y(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	2.861	9.088	4.113	0.856	0.588	−32.8
	Zr	3.331	9.643	4.066	0.859	0.583	−32.3
	Th	3.726	11.174	3.980	0.866	0.592	−32.4
	Pa	3.595	10.629	3.886	0.863	0.594	−35.0
	U	3.388	11.470	3.454	0.847	0.580	−9.7
	Np	3.906	8.972	4.009	0.865	0.593	16.6
	Pu	3.706	10.465	3.824	0.860	0.582	−2.9
	Nd	3.894	11.108	3.898	0.863	0.566	−12.2
Rh	Ti	2.946	9.596	4.347	0.853	0.593	−67.8
	Zr	3.220	10.086	4.483	0.859	0.593	−76.7
	Th	3.914	11.520	4.139	0.864	0.599	−90.4
	Pa	3.799	11.073	4.060	0.862	0.600	−70.5
	U	4.061	9.809	4.092	0.870	0.604	−34.4
	Np	3.787	10.474	4.161	0.865	0.600	−20.1
	Pu	3.791	10.759	4.111	0.860	0.592	−46.8
	Nd	3.936	11.128	4.100	0.862	0.589	−68.7
Ir	Ti	2.948	9.755	4.354	0.849	0.592	−76.6
	Zr	3.180	10.265	4.515	0.857	0.592	−84.4
	Th	3.936	11.414	4.212	0.863	0.598	−98.3
	Pa	3.815	11.093	4.115	0.862	0.600	−88.4
	U	3.848	10.785	4.030	0.865	0.602	−49.6
	Np	3.838	10.603	4.116	0.865	0.600	−31.5
	Pu	3.821	10.745	4.129	0.860	0.593	−52.8
	Nd	3.963	11.048	4.144	0.859	0.586	−66.0

Tabelle A.3.3: Ergebnisse der PBE-Strukturoptimierungen der MN-Verbindungen im FeB-Typ. Gitterparameter, x-, z-Lageparameter (Punktlage 4c) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalarrelativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	$x(M)$	$z(M)$	$x(N)$	$z(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	5.319	4.108	4.891	0.166	0.633	0.056	0.159	–
	Zr	6.102	4.216	5.067	0.177	0.637	0.044	0.154	−32.7
	Th	7.270	3.990	5.707	0.175	0.668	0.059	0.161	−29.5
	Pa	7.157	3.819	5.418	0.171	0.670	0.062	0.166	−35.2
	U	6.664	3.215	6.252	0.156	0.595	0.074	0.130	−9.2
	Np	4.296	4.296	6.075	0.000	0.625	0.000	0.125	−17.7
	Pu	7.052	3.820	5.541	0.179	0.640	0.045	0.142	−0.9
	Nd	7.605	4.166	5.436	0.175	0.604	0.032	0.087	−12.6
Rh	Ti	5.576	4.309	5.151	0.165	0.637	0.055	0.168	−67.9
	Zr	6.153	4.490	5.293	0.176	0.641	0.047	0.169	−78.7
	Th	7.632	4.166	5.879	0.171	0.668	0.067	0.173	−87.9
	Pa	7.625	3.906	5.752	0.168	0.669	0.071	0.175	−69.7
	U	4.638	4.614	6.517	−0.001	0.626	0.015	0.124	−57.9
	Np	6.318	4.661	5.509	0.174	0.642	0.054	0.167	−17.2
	Pu	7.166	4.198	5.570	0.179	0.645	0.048	0.165	−44.9
	Nd	7.164	4.574	5.530	0.185	0.632	0.037	0.158	−66.6
Ir	Ti	5.225	4.408	5.361	0.139	0.627	0.083	0.148	−77.4
	Zr	6.141	4.476	5.416	0.174	0.640	0.045	0.170	−86.0
	Th	7.634	4.291	5.792	0.171	0.665	0.065	0.172	−96.0
	Pa	7.579	4.049	5.688	0.169	0.670	0.071	0.177	−87.1
	U	7.485	4.062	5.522	0.168	0.664	0.071	0.177	−47.4
	Np	7.289	4.185	5.494	0.177	0.662	0.059	0.175	−29.0
	Pu	7.279	4.168	5.602	0.176	0.651	0.053	0.165	−50.4
	Nd	7.252	4.579	5.518	0.184	0.620	0.033	0.139	−65.2

Tabelle A.3.4: Ergebnisse der PBE-Strukturoptimierungen der MN-Verbindungen im TiNi-Typ. Gitterparameter, x-, z-Lageparameter (Punktlage $4e$) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalarrelativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	β / °	$x(M)$	$z(M)$	$x(N)$	$z(N)$	$\Delta H/\frac{\mathrm{kJ}}{\mathrm{mol}}$
Co	Ti	5.153	4.214	2.967	125.22	0.250	0.249	0.750	0.250	−36.4
	Zr	5.505	4.496	3.179	125.30	0.250	0.251	0.752	0.252	−27.9
	Th	5.563	5.572	3.931	134.92	0.249	−0.001	0.749	−0.001	−21.6
	Pa	5.392	5.308	3.655	132.61	0.250	0.000	0.750	0.000	−27.9
	U	5.301	5.156	3.422	129.88	0.250	0.000	0.750	0.000	7.8
	Np	5.800	4.905	2.905	124.32	0.237	0.192	0.725	0.249	5.5
	Pu	5.565	4.723	3.256	121.78	0.229	0.265	0.702	0.195	−1.7
	Nd	5.710	5.115	3.094	122.48	0.248	0.054	0.746	0.049	–
Rh	Ti	5.475	4.437	2.925	122.04	0.272	0.270	0.785	0.288	−71.0
	Zr	5.763	4.662	3.117	121.45	0.235	0.243	0.713	0.206	−73.9
	Th	5.788	5.799	4.072	134.56	0.252	0.002	0.752	0.003	−84.9
	Pa	5.644	5.593	3.871	133.22	0.250	0.001	0.749	0.001	−65.6
	U	5.961	5.254	2.937	119.34	0.250	0.010	0.750	0.013	−23.9
	Np	5.894	4.816	3.367	124.49	0.234	0.231	0.720	0.221	−20.3
	Pu	5.841	4.864	3.402	123.91	0.250	0.253	0.750	0.249	−43.7
	Nd	5.541	5.565	3.707	96.87	0.256	0.012	0.745	0.011	−62.1
Ir	Ti	5.448	4.460	2.919	120.46	0.223	0.243	0.707	0.186	−81.4
	Zr	5.533	4.556	3.155	112.30	0.218	0.325	0.687	0.117	−84.6
	Th	5.837	5.838	4.126	134.97	0.250	0.000	0.750	0.000	−92.8
	Pa	5.667	5.665	3.960	134.37	0.250	0.001	0.750	0.001	−83.4
	U	5.599	5.596	3.942	134.82	0.251	0.001	0.751	0.001	−41.4
	Np	5.865	4.889	3.073	117.62	0.214	0.247	0.692	0.187	−27.1
	Pu	5.952	5.083	3.078	120.68	0.240	0.242	0.733	0.231	−46.0
	Nd	5.582	5.499	2.951	110.35	0.240	0.018	0.761	0.020	−60.7

A.3.2 Optimierte Strukturen der *MN*-Verbindungen mit dem LDA-PW-Funktional

Tabelle A.3.5: Ergebnisse der LDA-PW-Strukturoptimierungen der MN-Verbindungen im CsCl-, NaTl- und UCo-Typ. Gitterparameter, Lageparameter vom UCo-Typ (Punktlage $8a$) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

N	M	CsCl-Typ		NaTl-Typ		UCo-Typ			
		a/Å	$\Delta H/\frac{\text{kJ}}{\text{mol}}$	a/Å	$\Delta H/\frac{\text{kJ}}{\text{mol}}$	a/Å	$x(M)$	$x(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	2.904	−43.0	5.752	−21.9	5.808	0.000	0.250	−43.0
	Zr	3.106	−32.2	6.109	−2.6	6.213	0.000	0.250	−32.2
	Th	3.373	−7.9	6.595	20.8	6.698	0.013	0.290	−14.9
	Pa	3.229	−12.0	6.285	−31.0	6.355	0.028	0.295	−39.4
	U	3.130	13.0	6.091	−32.0	6.175	0.035	0.298	−29.6
	Np	3.139	49.1	5.940	−24.3	6.046	0.047	0.307	−7.0
	Pu	3.178	39.4	5.886	−12.7	5.987	0.056	0.312	1.7
	Nd	3.241	−5.7	6.219	−19.8	6.356	0.035	0.309	−15.1
Rh	Ti	3.044	−70.4	6.070	−44.4	6.088	0.000	0.250	−70.5
	Zr	3.227	−72.8	6.368	−45.8	6.454	0.000	0.250	−72.8
	Th	3.487	−62.4	6.792	−41.7	6.935	0.015	0.282	−65.2
	Pa	3.364	−48.0	6.536	−69.9	6.629	0.033	0.289	−67.5
	U	3.284	−11.3	6.381	−55.6	6.470	0.042	0.293	−41.6
	Np	3.312	17.6	6.255	−33.8	6.354	0.055	0.300	−12.9
	Pu	3.324	−1.5	6.211	−16.8	6.579	0.027	0.284	−3.6
	Nd	3.373	−54.1	6.506	−57.6	6.744	−0.003	0.244	−54.0
Ir	Ti	3.066	−76.4	6.128	−49.0	6.133	0.007	0.260	−77.2
	Zr	3.249	−77.1	6.412	−48.3	6.501	0.004	0.259	−77.2
	Th	3.510	−64.9	6.827	−38.6	6.995	0.013	0.278	−67.0
	Pa	3.396	−54.0	6.594	−69.7	6.686	0.033	0.288	−72.4
	U	3.321	−17.3	6.458	−53.7	6.533	0.043	0.292	−48.2
	Np	3.339	12.0	6.348	−29.6	6.425	0.055	0.299	−17.1
	Pu	3.348	−3.9	6.304	−12.5	6.638	0.025	0.282	−5.8
	Nd	3.392	−53.8	6.567	−53.2	6.784	0.000	0.250	−53.8

Tabelle A.3.6: Ergebnisse der LDA-PW-Strukturoptimierungen der MN-Verbindungen im CrB-Typ. Gitterparameter, y-Lageparameter (Punktlage 4c) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	$y(M)$	$y(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	2.790	8.854	4.025	0.856	0.589	−40.4
	Zr	3.261	9.444	3.966	0.859	0.583	−38.5
	Th	3.661	10.911	3.850	0.867	0.593	−37.1
	Pa	3.549	10.414	3.747	0.862	0.594	−36.7
	U	3.300	11.214	3.352	0.844	0.579	−9.4
	Np	4.309	7.659	3.685	0.888	0.605	17.2
	Pu	3.558	10.151	3.636	0.862	0.587	29.6
	Nd	3.633	10.927	3.543	0.863	0.582	−11.6
Rh	Ti	2.878	9.390	4.265	0.853	0.593	−69.2
	Zr	3.140	9.916	4.402	0.859	0.593	−76.9
	Th	3.847	11.226	4.056	0.864	0.599	−86.9
	Pa	3.764	10.801	3.958	0.862	0.600	−63.2
	U	4.280	8.677	3.995	0.889	0.612	−24.3
	Np	3.844	10.013	3.939	0.866	0.601	15.3
	Pu	3.677	10.376	4.017	0.861	0.594	−4.7
	Nd	3.803	10.661	3.955	0.861	0.593	−55.2
Ir	Ti	2.888	9.562	4.286	0.850	0.592	−77.8
	Zr	3.112	10.089	4.450	0.857	0.592	−84.3
	Th	3.877	11.172	4.133	0.863	0.598	−93.9
	Pa	3.767	10.878	4.033	0.862	0.600	−79.7
	U	3.830	10.499	3.912	0.865	0.603	−30.4
	Np	3.790	10.356	3.965	0.865	0.601	3.5
	Pu	3.718	10.441	4.041	0.861	0.595	−11.7
	Nd	3.819	10.643	4.041	0.861	0.591	−55.9

Tabelle A.3.7: Ergebnisse der LDA-PW-Strukturoptimierungen der MN-Verbindungen im FeB-Typ. Gitterparameter, x-,z-Lageparameter (Punktlage 4c) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	$x(M)$	$z(M)$	$x(N)$	$z(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	5.193	4.015	4.768	0.167	0.633	0.055	0.160	−42.1
	Zr	5.983	4.116	4.948	0.177	0.638	0.043	0.154	−38.7
	Th	7.218	3.810	5.577	0.173	0.674	0.062	0.161	−34.5
	Pa	7.153	3.575	5.406	0.170	0.669	0.060	0.164	−37.6
	U	6.518	3.138	6.109	0.154	0.595	0.075	0.128	−10.0
	Np	6.426	3.001	6.181	0.141	0.581	0.080	0.122	21.7
	Pu	6.816	3.684	5.230	0.178	0.648	0.049	0.154	32.4
	Nd	7.422	4.343	4.404	0.166	0.535	0.045	0.064	−15.8
Rh	Ti	5.206	4.267	5.158	0.149	0.629	0.076	0.152	−69.4
	Zr	6.008	4.403	5.208	0.175	0.641	0.047	0.168	−78.9
	Th	7.537	4.045	5.757	0.171	0.669	0.067	0.172	−84.4
	Pa	7.525	3.815	5.616	0.168	0.667	0.071	0.173	−62.7
	U	4.507	4.503	6.368	0.000	0.625	0.000	0.125	−55.2
	Np	4.427	4.423	6.250	0.000	0.625	0.000	0.125	−34.2
	Pu	6.907	4.128	5.374	0.178	0.647	0.051	0.166	−2.2
	Nd	7.164	4.053	5.519	0.180	0.645	0.052	0.166	−53.5
Ir	Ti	5.206	4.267	5.158	0.149	0.629	0.076	0.152	−69.4
	Zr	6.008	4.403	5.208	0.175	0.641	0.047	0.168	−78.9
	Th	7.537	4.045	5.757	0.171	0.669	0.067	0.172	−84.4
	Pa	7.525	3.815	5.616	0.168	0.667	0.071	0.173	−62.7
	U	4.507	4.503	6.368	0.000	0.625	0.000	0.125	−55.2
	Np	4.427	4.423	6.250	0.000	0.625	0.000	0.125	−34.2
	Pu	6.907	4.128	5.374	0.178	0.647	0.051	0.166	−2.2
	Nd	7.164	4.053	5.519	0.180	0.645	0.052	0.166	−53.5

Tabelle A.3.8: Ergebnisse der LDA-PW-Strukturoptimierungen der MN-Verbindungen im TiNi-Typ. Gitterparameter, x-, z-Lageparameter (Punktlage 4e) und Bildungsenthalpie ΔH pro Atom. PBE-Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

N	M	a/Å	b/Å	c/Å	β / °	$x(M)$	$z(M)$	$x(N)$	$z(N)$	$\Delta H/\frac{\text{kJ}}{\text{mol}}$
Co	Ti	4.988	4.059	2.757	117.94	0.271	0.218	0.802	0.334	−42.7
	Zr	5.375	4.395	3.106	125.18	0.249	0.249	0.748	0.248	−32.4
	Th	5.420	5.425	3.835	135.05	0.248	−0.001	0.749	0.000	−27.4
	Pa	5.255	5.207	3.584	132.94	0.250	0.002	0.750	0.002	−31.0
	U	5.193	5.049	3.346	130.33	0.250	1.001	0.750	0.001	11.9
	Np	5.584	4.753	2.416	115.55	0.250	−0.001	0.750	0.001	41.5
	Pu	5.484	4.585	2.879	120.78	0.203	0.130	0.667	0.187	6.2
	Nd	5.425	4.861	2.690	112.28	0.250	0.010	0.749	0.015	0.6
Rh	Ti	5.385	4.336	2.855	122.34	0.227	0.221	0.715	0.220	−72.3
	Zr	5.584	4.600	3.179	124.54	0.251	0.250	0.752	0.253	−73.4
	Th	5.653	5.686	3.972	134.35	0.252	0.003	0.752	0.003	−80.4
	Pa	5.534	5.486	3.786	133.10	0.250	0.000	0.750	0.001	−58.2
	U	5.888	5.071	2.799	118.30	0.251	0.001	0.750	0.001	−7.5
	Np	5.697	4.332	2.823	111.20	0.125	0.077	0.616	0.249	−17.1
	Pu	5.717	4.894	2.987	119.50	0.231	0.231	0.720	0.216	−2.5
	Nd	5.841	4.850	3.258	123.87	0.248	0.249	0.745	0.243	−54.3
Ir	Ti	5.391	4.382	2.863	121.45	0.278	0.272	0.790	0.298	−82.9
	Zr	5.650	4.514	3.398	127.01	0.250	0.250	0.751	0.201	−78.2
	Th	5.729	5.730	4.048	134.94	0.252	0.004	0.752	0.003	−87.7
	Pa	5.567	5.564	3.883	134.23	0.249	−0.001	0.749	−0.001	−74.9
	U	5.488	5.490	3.859	134.72	0.254	0.010	0.753	0.008	−21.8
	Np	6.025	4.325	2.849	117.80	0.139	0.138	0.652	0.158	−9.8
	Pu	5.973	5.024	2.903	122.04	0.235	0.224	0.727	0.248	−7.3
	Nd	–	–	–	–	–	–	–	–	–

A.3.3 Optimierte Elementstrukturen mit GGA-PBE und LDA-PW-Funktional

Tabelle A.3.9: Ergebnisse der DFT-Strukturoptimierungen der Elementstrukturen. Raumgruppe, Pearson-Symbol und Gitterparameter. Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

		Ti	Zr	Nd	Th	Pa	U	Np	Pu	Co	Rh	Ir
GGA-PBE	Raumgruppe	$P6_3/mmc$	$P6_3/mmc$	$P6_3/mmc$	$Fm\bar{3}m$	$I4/mmm$	$Cmcm$	$Pnma$	$P2_1/m$	$P6_3/mmc$	$Fm\bar{3}m$	$Fm\bar{3}m$
	Pearson-Symbol	$hP2$	$hP2$	$hP2$	$cF4$	$tI2$	$oS4$	$oP8$	$mP16$	$hP2$	$cF4$	$cF4$
	a / Å	2.940	3.232	3.641	3.567	3.941	2.805	6.574	5.995	2.458	2.706	2.745
	b / Å	–	–	–	–	–	5.832	4.668	4.536	–	–	–
	c / Å	4.654	5.167	12.144	–	3.198	4.901	4.788	10.952	3.966	–	–
	β / °	–	–	–	–	–	–	–	101.68	–	–	–
LDA-PW	a / Å	2.865	3.147	3.072	4.902	3.851	2.726	6.450	5.797	2.434	3.751	3.823
	b / Å	–	–	–	–	–	5.716	4.572	4.376	–	–	–
	c / Å	4.536	5.083	11.432	–	3.119	4.820	4.681	10.641	3.925	–	–
	β / °	–	–	–	–	–	–	–	102.35	–	–	–

Tabelle A.3.10: Ergebnisse der DFT-Strukturoptimierungen der Elementstrukturen: Wyckoff-Position (WP), Atompositionen x, y und z der Atome M. Rechnungen mit skalar-relativistischer PAW-Basis mit Spinpolarisation.

Methode	Element (WP)	Koordinate	$M1$	$M2$	$M3$	$M4$	$M5$	$M6$	$M7$	$M8$
GGA-PBE	Pu (2e)	x	0.056	0.165	0.197	0.397	0.490	0.634	0.754	0.846
		y	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
		z	0.365	0.841	0.072	0.677	0.381	0.108	0.829	0.535
	Np (4c)	x	0.046	0.317						
		y	1/4	1/4						
		z	0.281	0.637						
	U (4c)	x	0							
		y	0.902							
		z	3/4							
LDA-PW	Pu (2e)	x	0.059	0.171	0.213	0.399	0.480	0.633	0.752	0.852
		y	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
		z	0.364	0.841	0.072	0.673	0.383	0.110	0.831	0.536
	Np (4c)	x	0.044	0.320						
		y	1/4	1/4						
		z	0.285	0.642						
	U (4c)	x	0							
		y	0.903							
		z	3/4							

A.3.4 PBE-Elektronenstrukturen der *MN*-Verbindungen

A.3.4.1 Elektronenstrukturen für *N* = Co

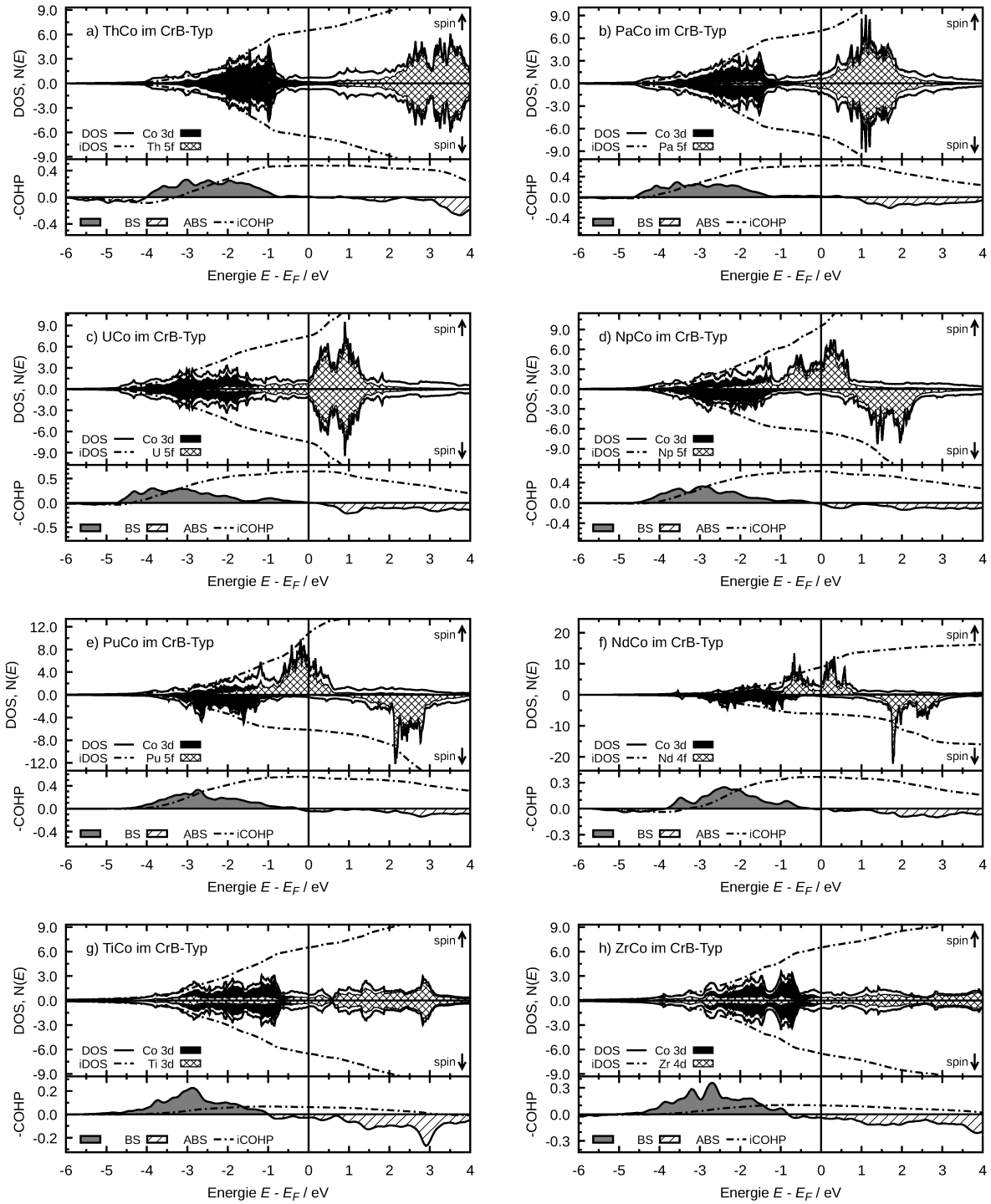

Abbildung A.3.1: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CrB-Typ für $N =$ Co und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

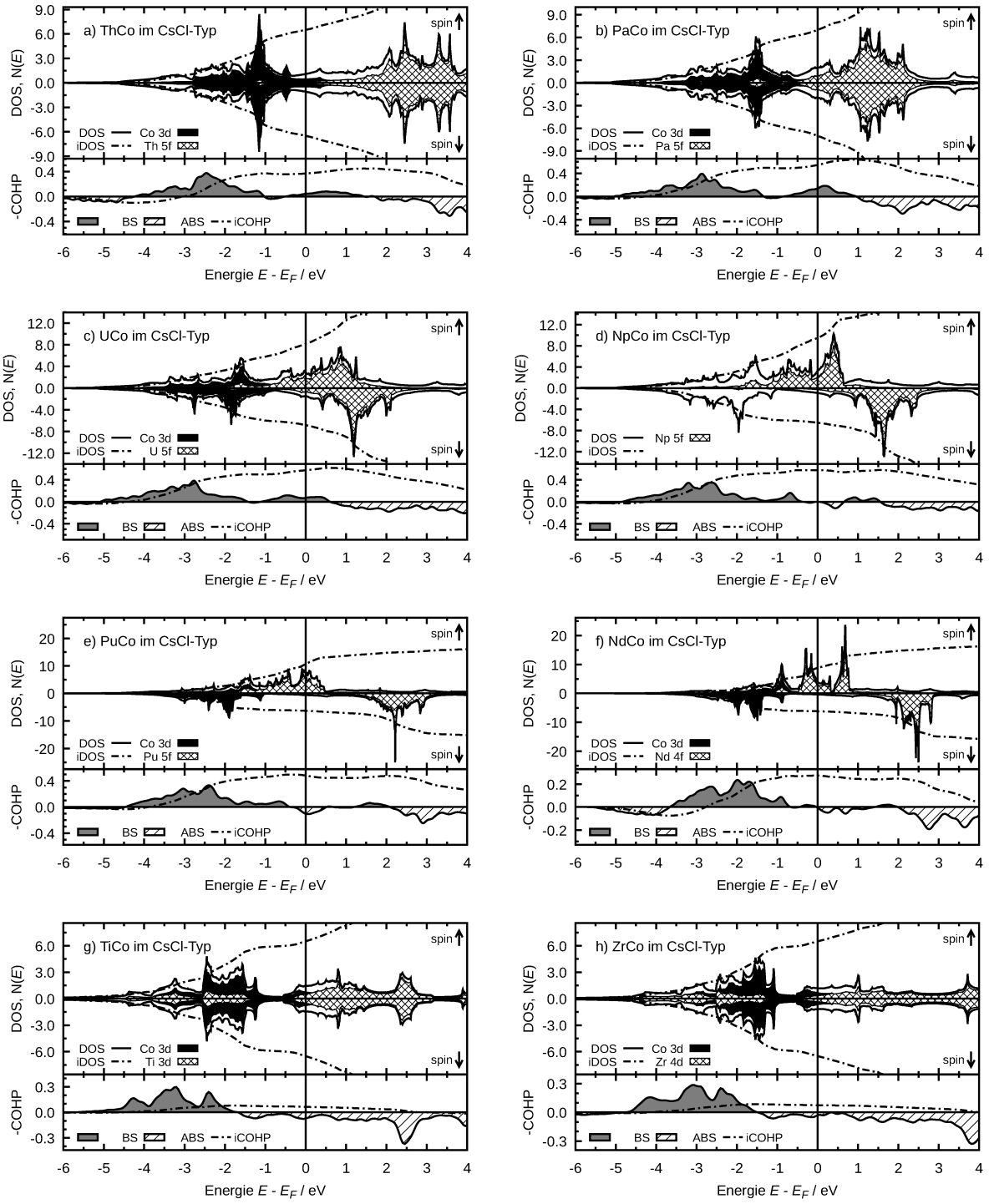

Abbildung A.3.2: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CsCl-Typ für $N = \mathrm{Co}$ und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

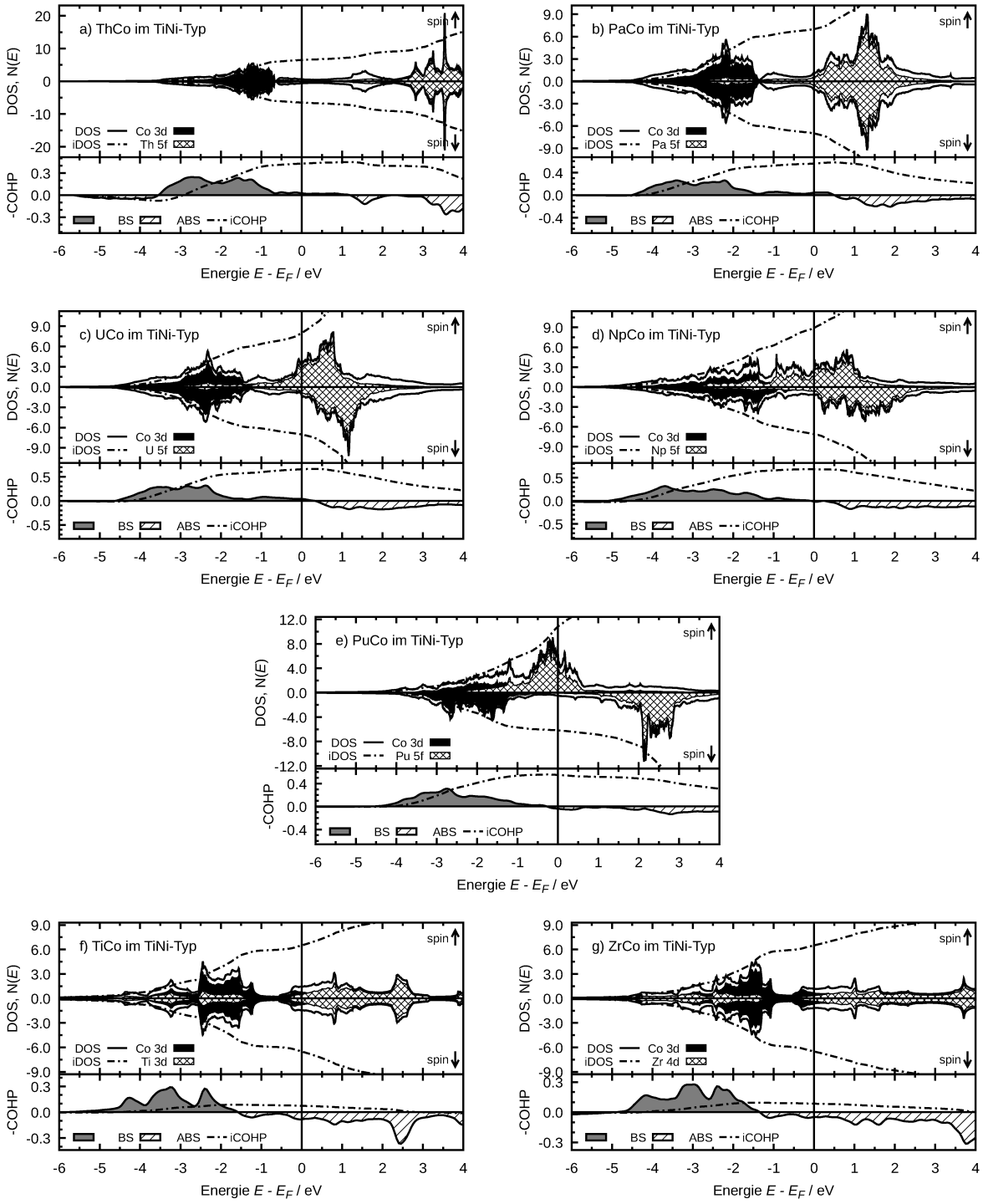

Abbildung A.3.3: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im TiNi-Typ für $N =$ Co und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Ti und **(g)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

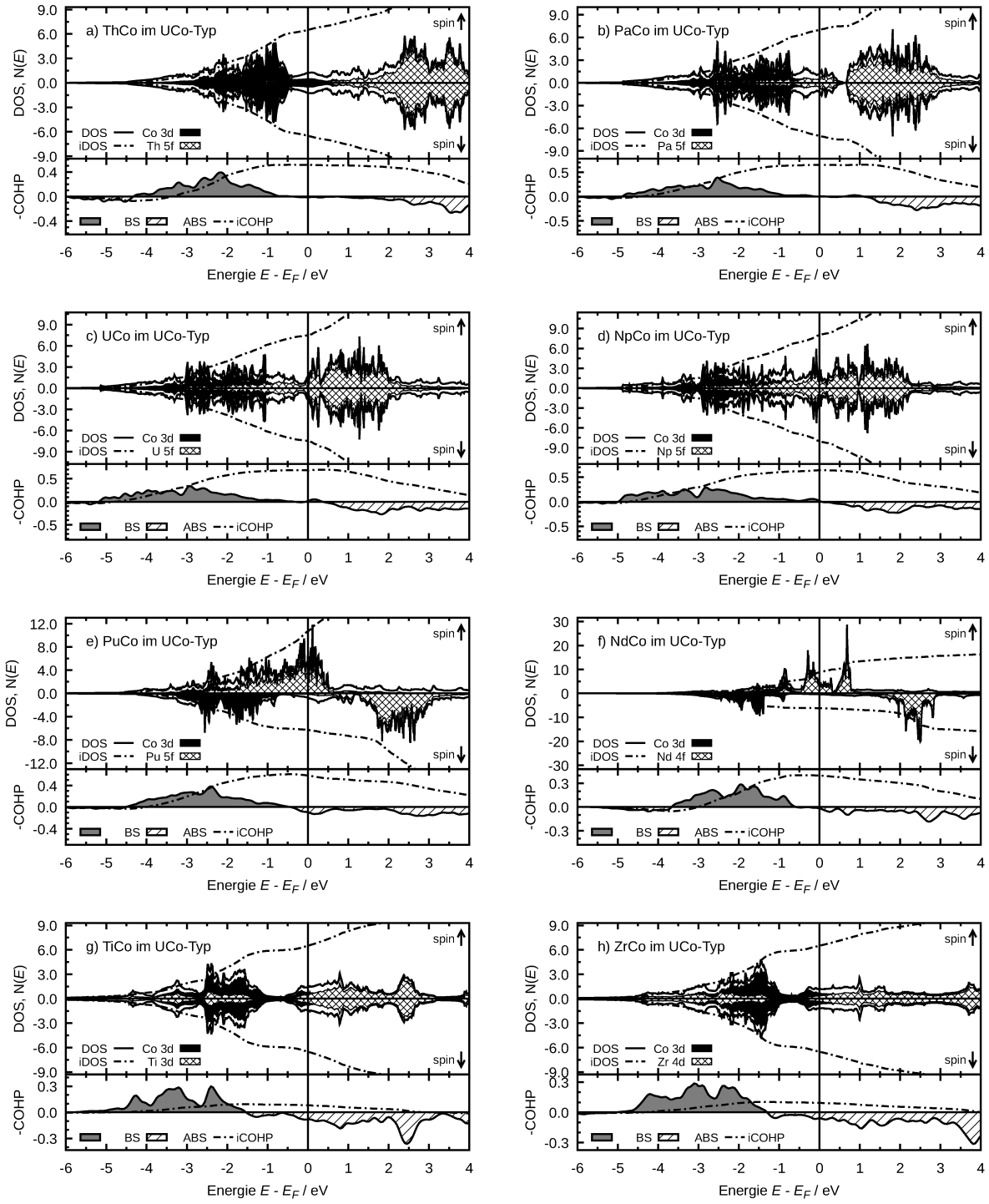

Abbildung A.3.4: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im UCo-Typ für $N =$ Co und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

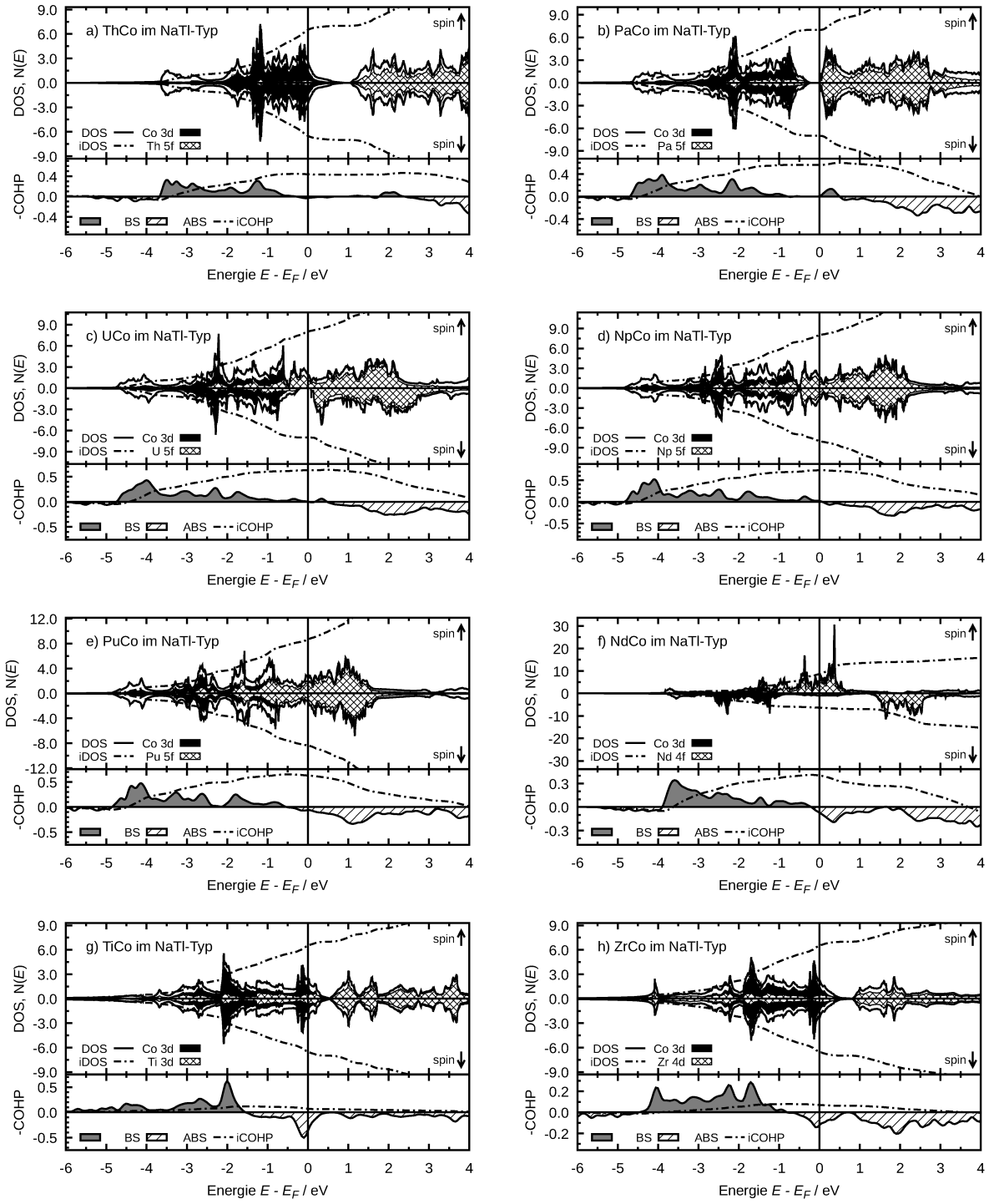

Abbildung A.3.5: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im NaTl-Typ für $N = \mathrm{Co}$ und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

A.3.4.2 Elektronenstrukturen für N = Rh

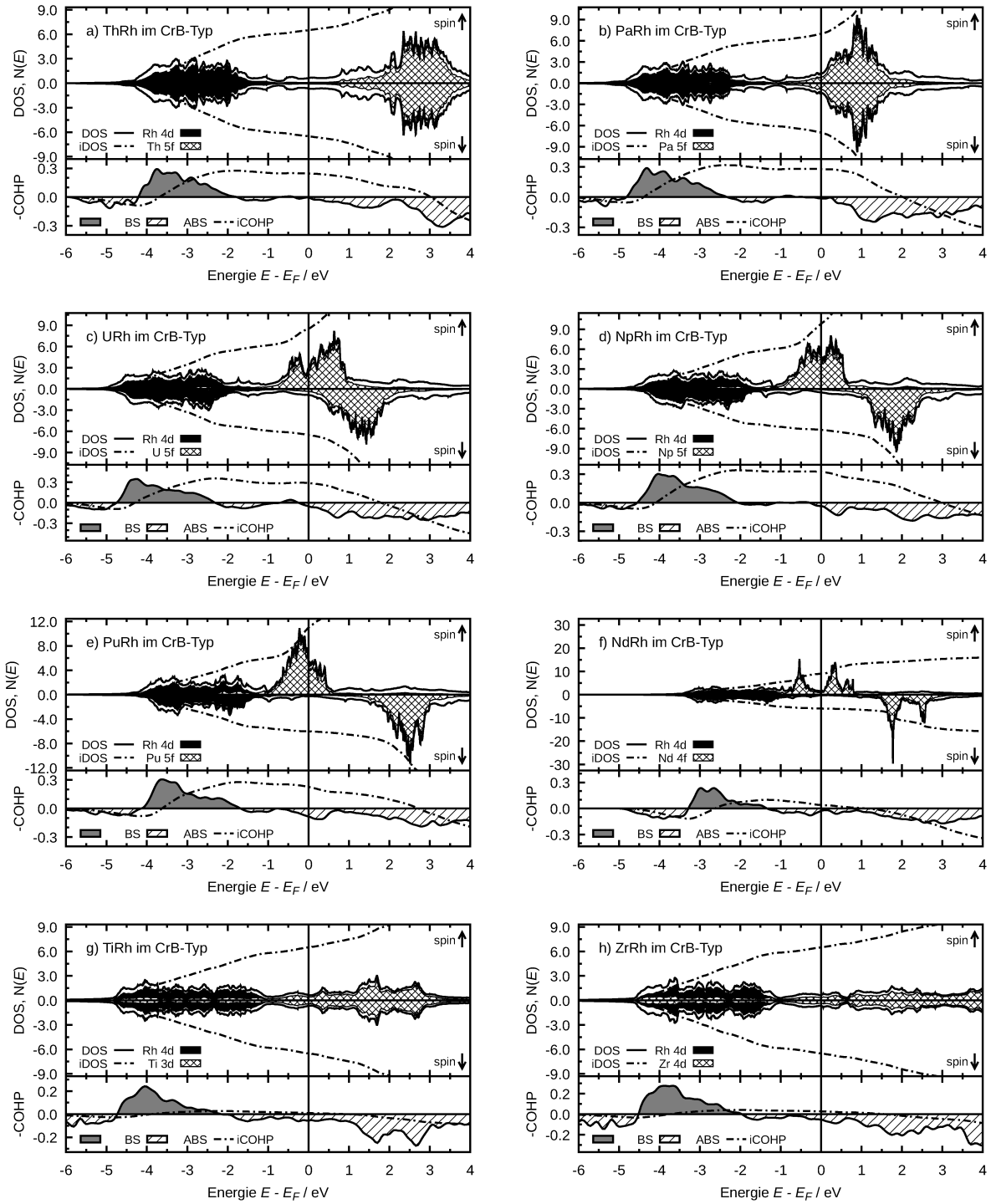

Abbildung A.3.6: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CrB-Typ für N = Rh und M = **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

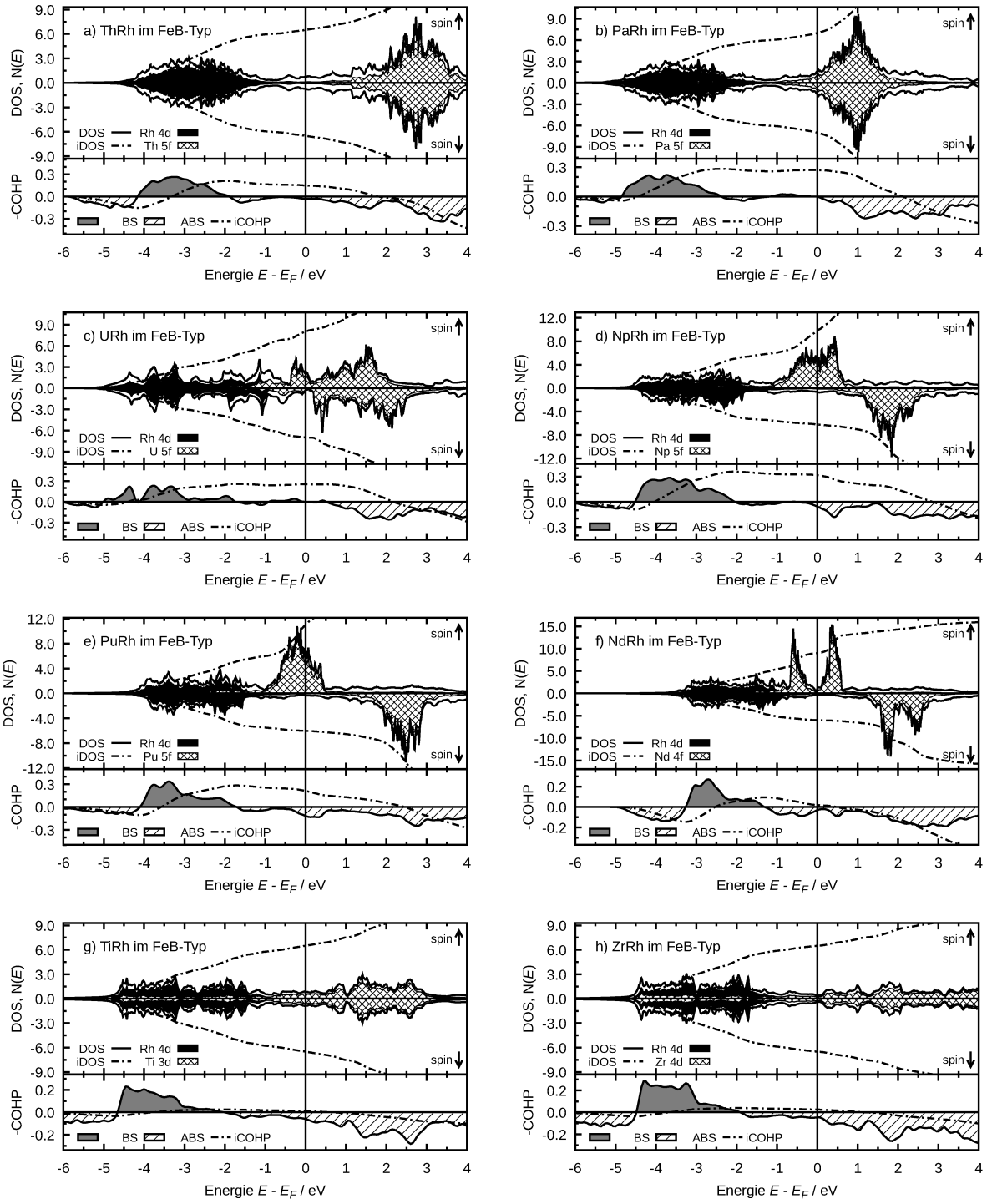

Abbildung A.3.7: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im FeB-Typ für $N =$ Rh und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

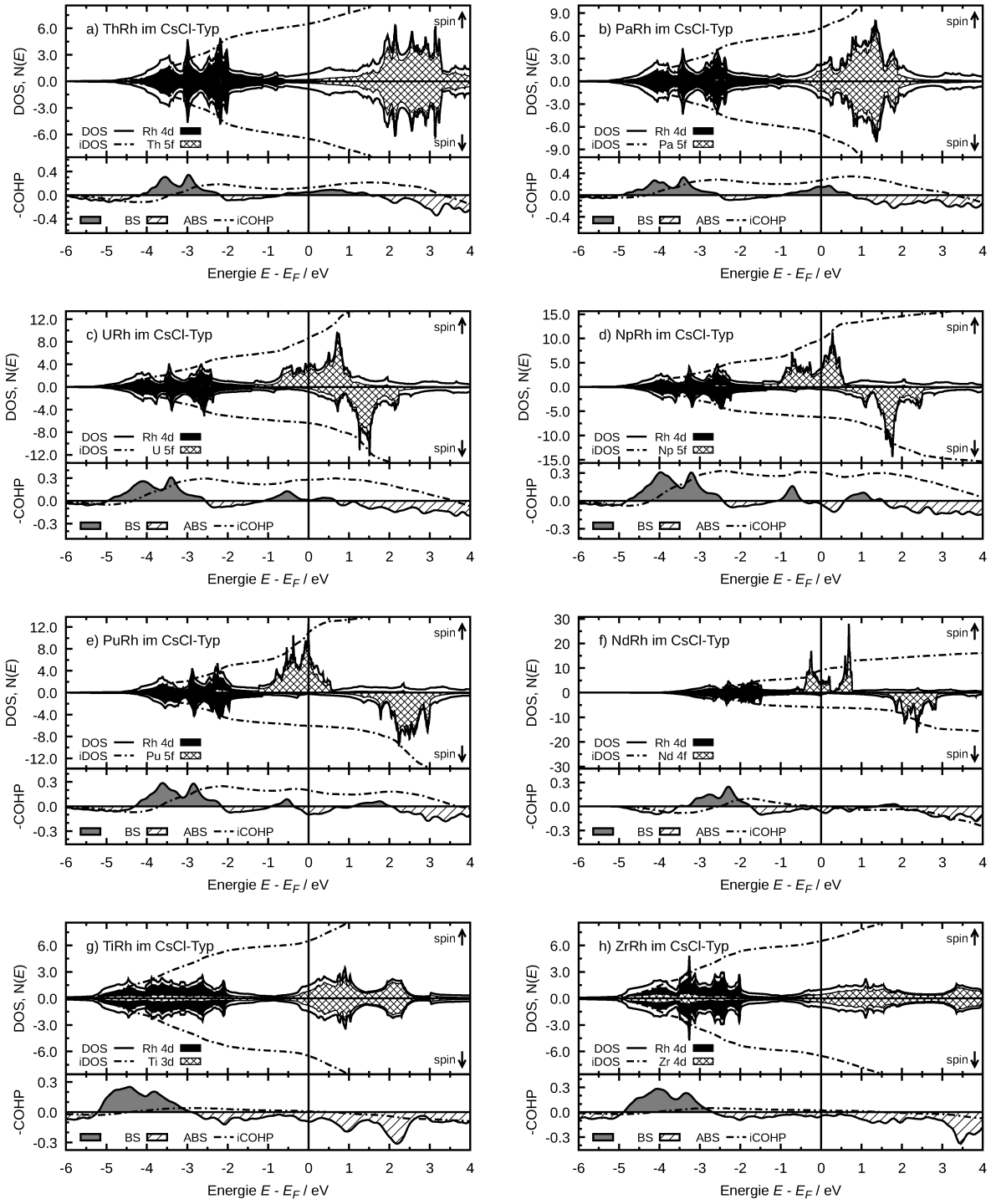

Abbildung A.3.8: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CsCl-Typ für $N =$ Rh und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

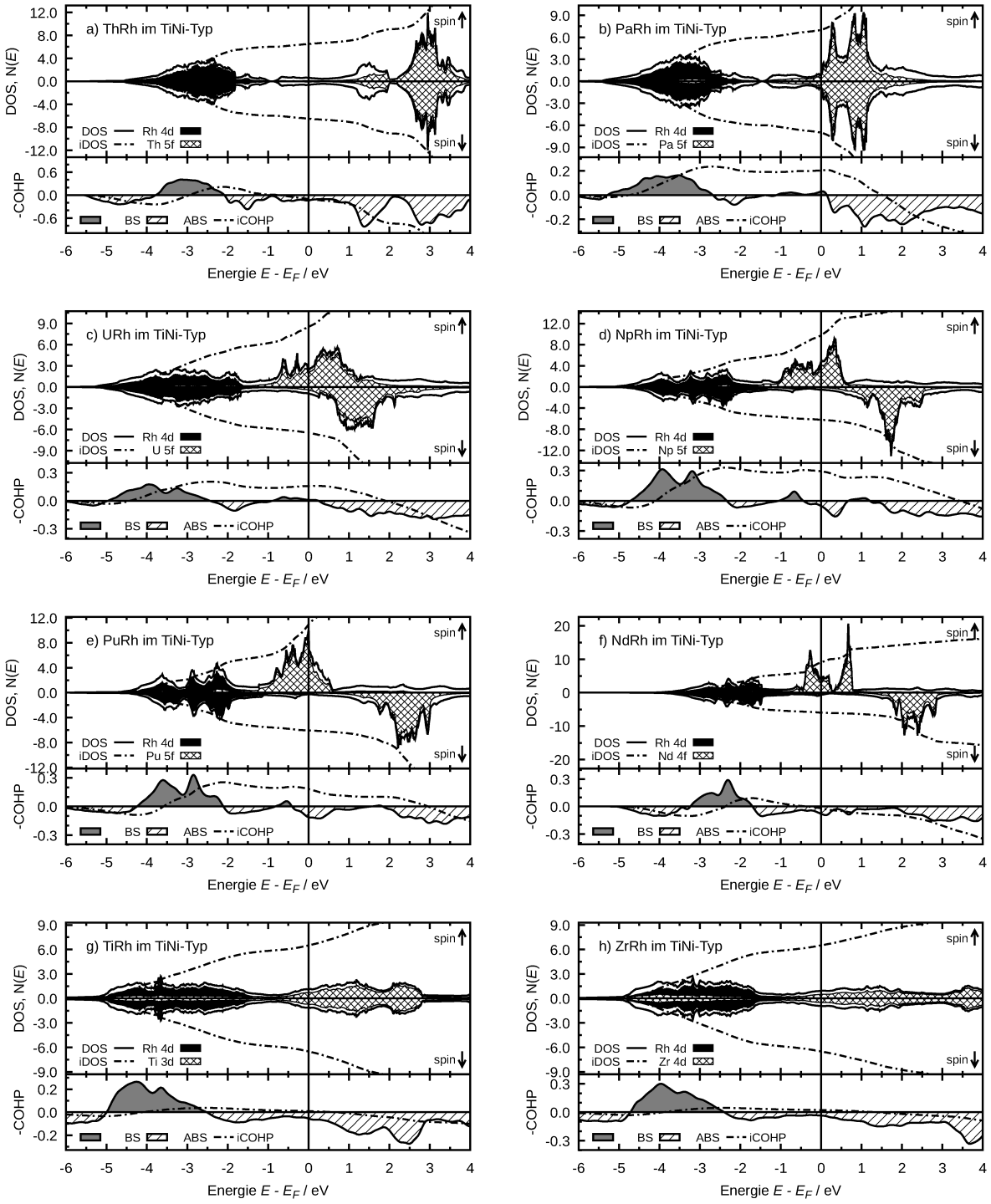

Abbildung A.3.9: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im TiNi-Typ für $N =$ Rh und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

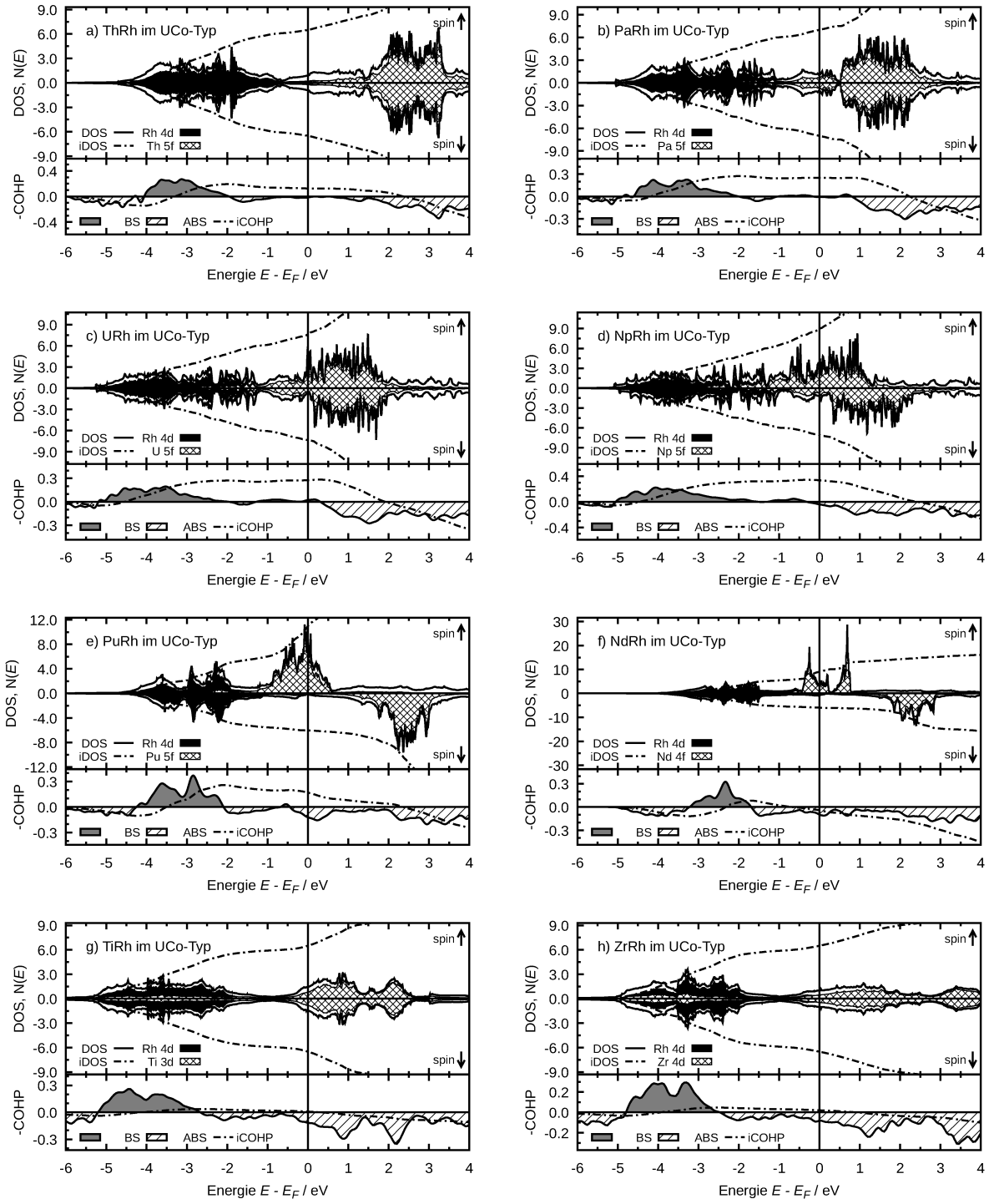

Abbildung A.3.10: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im UCo-Typ für $N =$ Rh und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

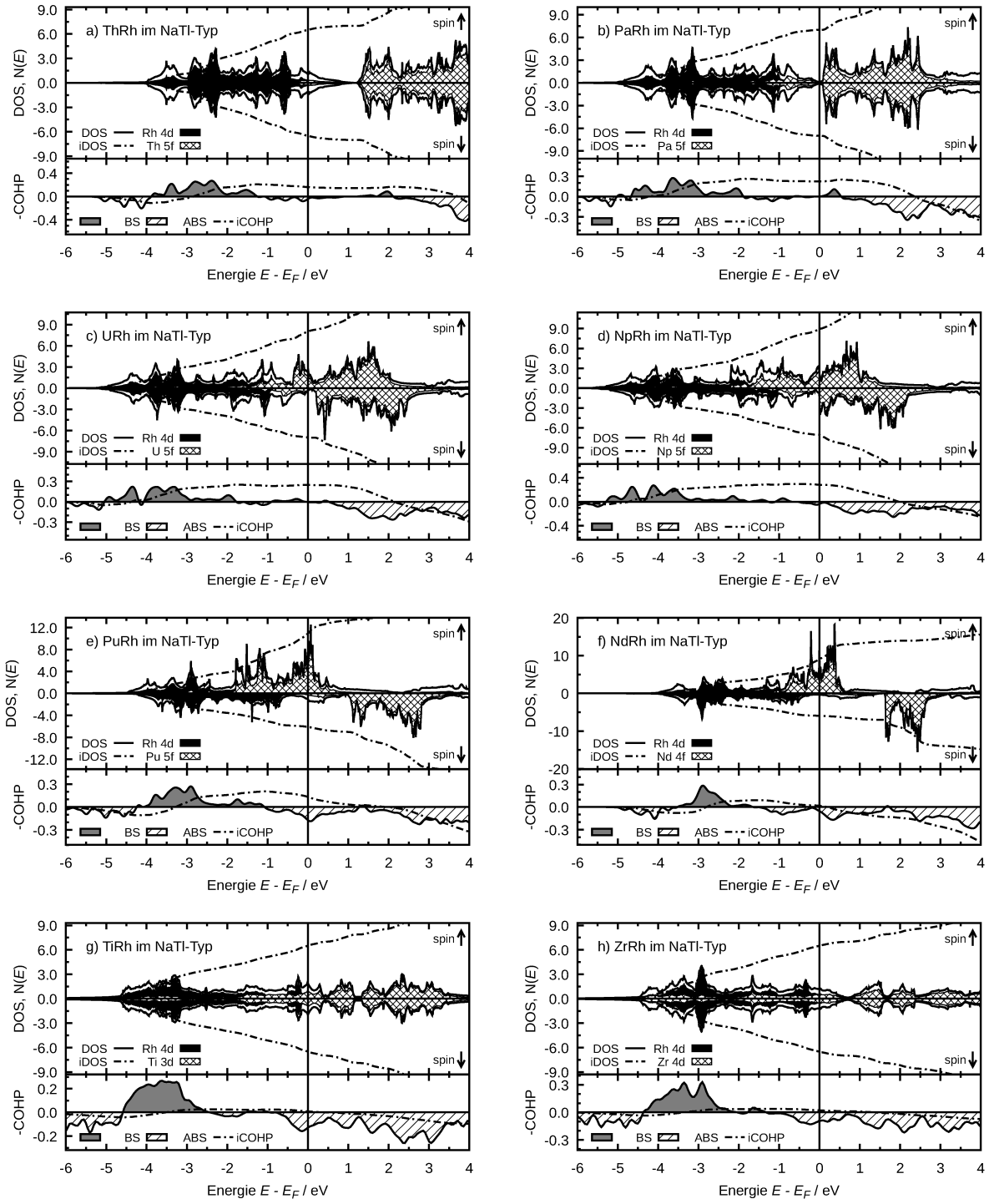

Abbildung A.3.11: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im NaTl-Typ für $N =$ Rh und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

A.3.4.3 Elektronenstrukturen für N = Ir

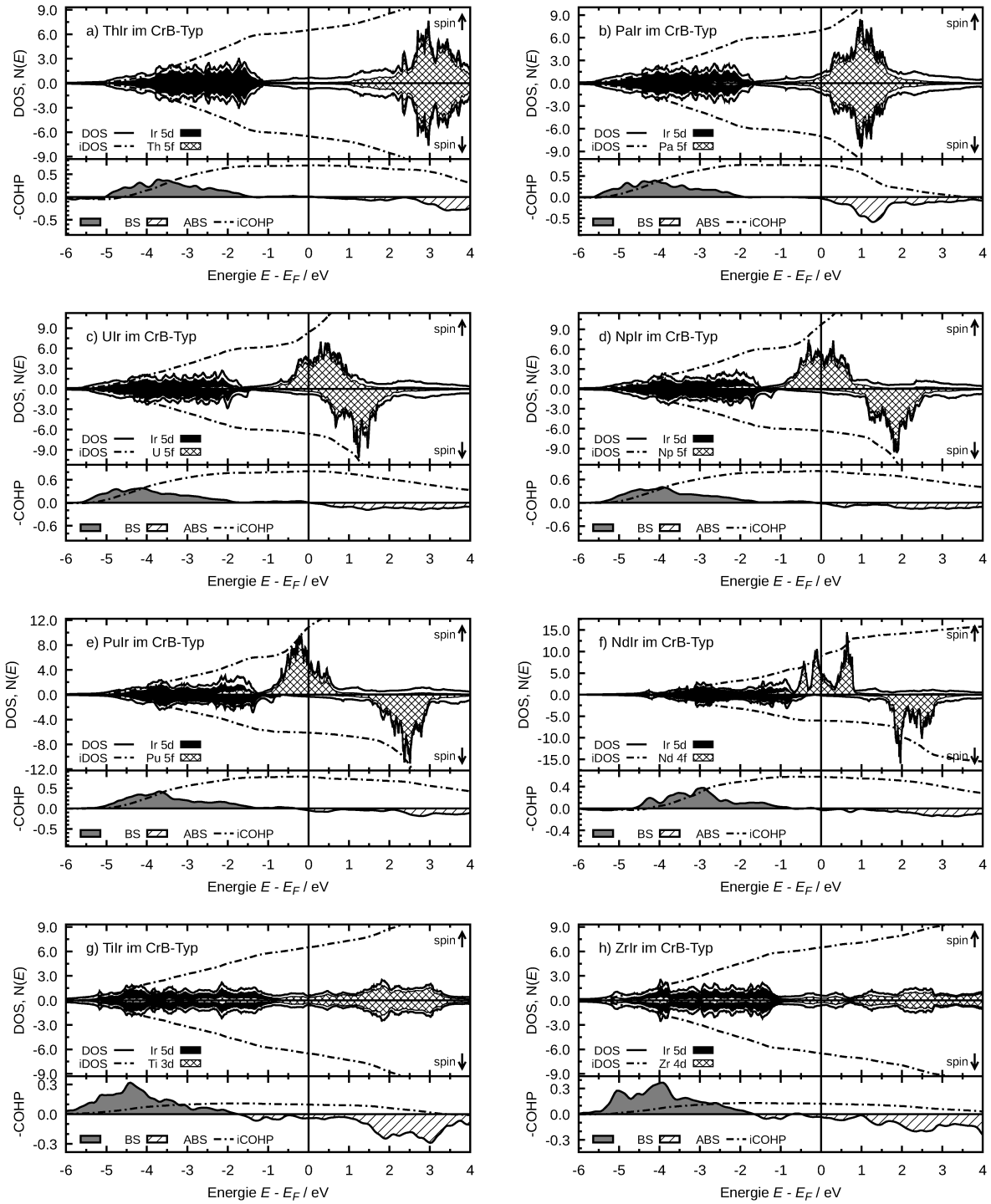

Abbildung A.3.12: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CrB-Typ für N = Ir und M = **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

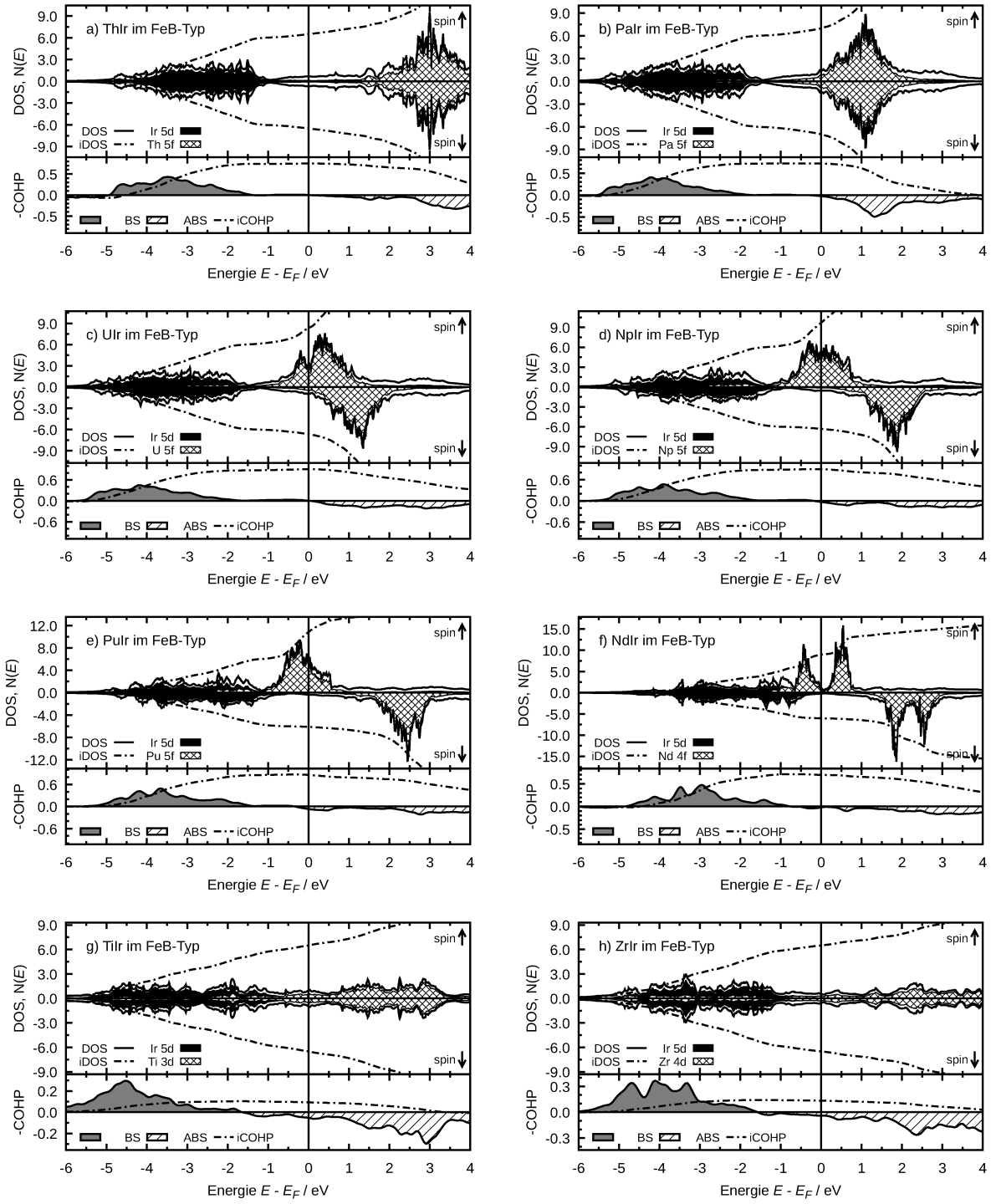

Abbildung A.3.13: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im FeB-Typ für $N =$ Ir und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

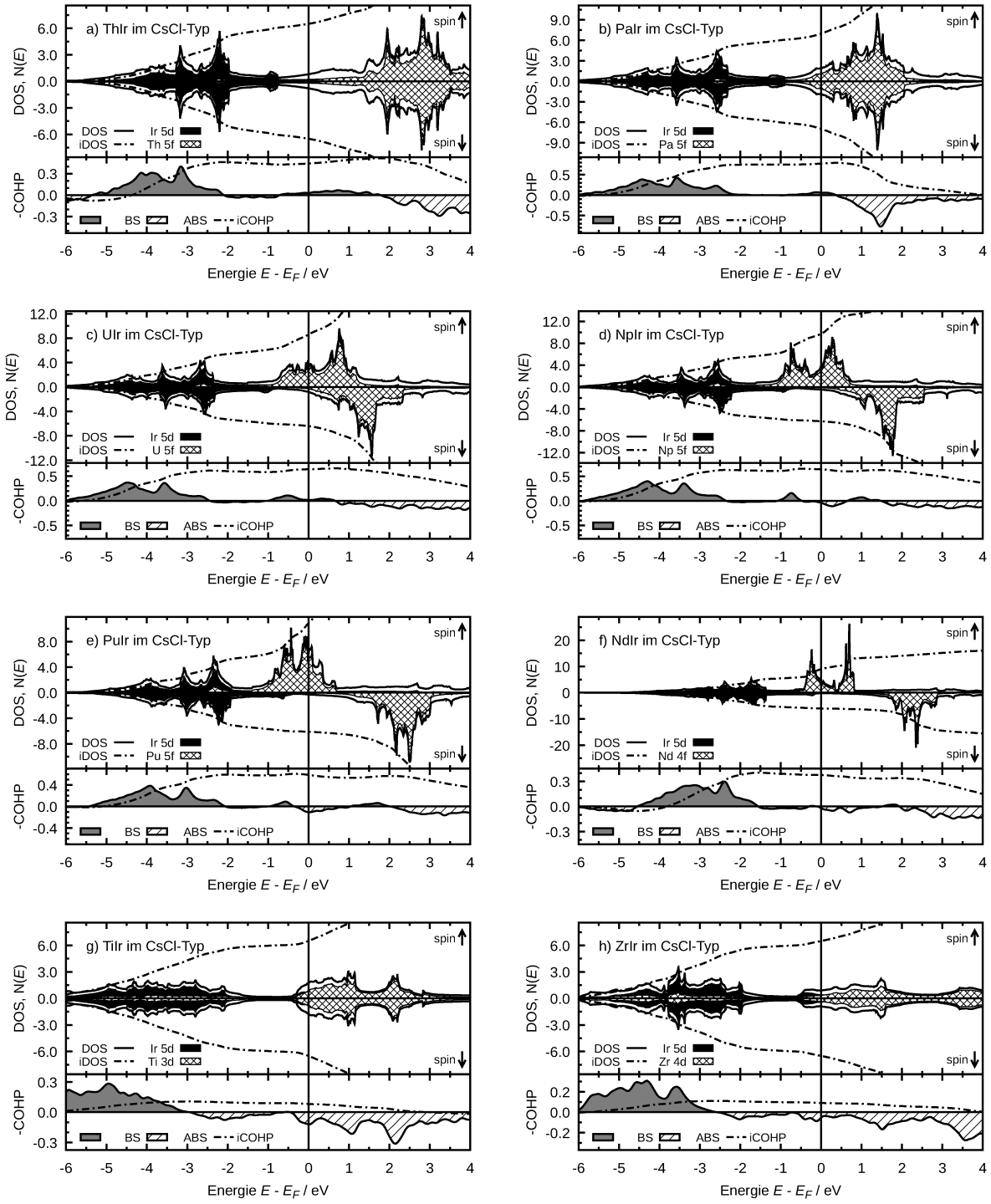

Abbildung A.3.14: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im CsCl-Typ für $N =$ Ir und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

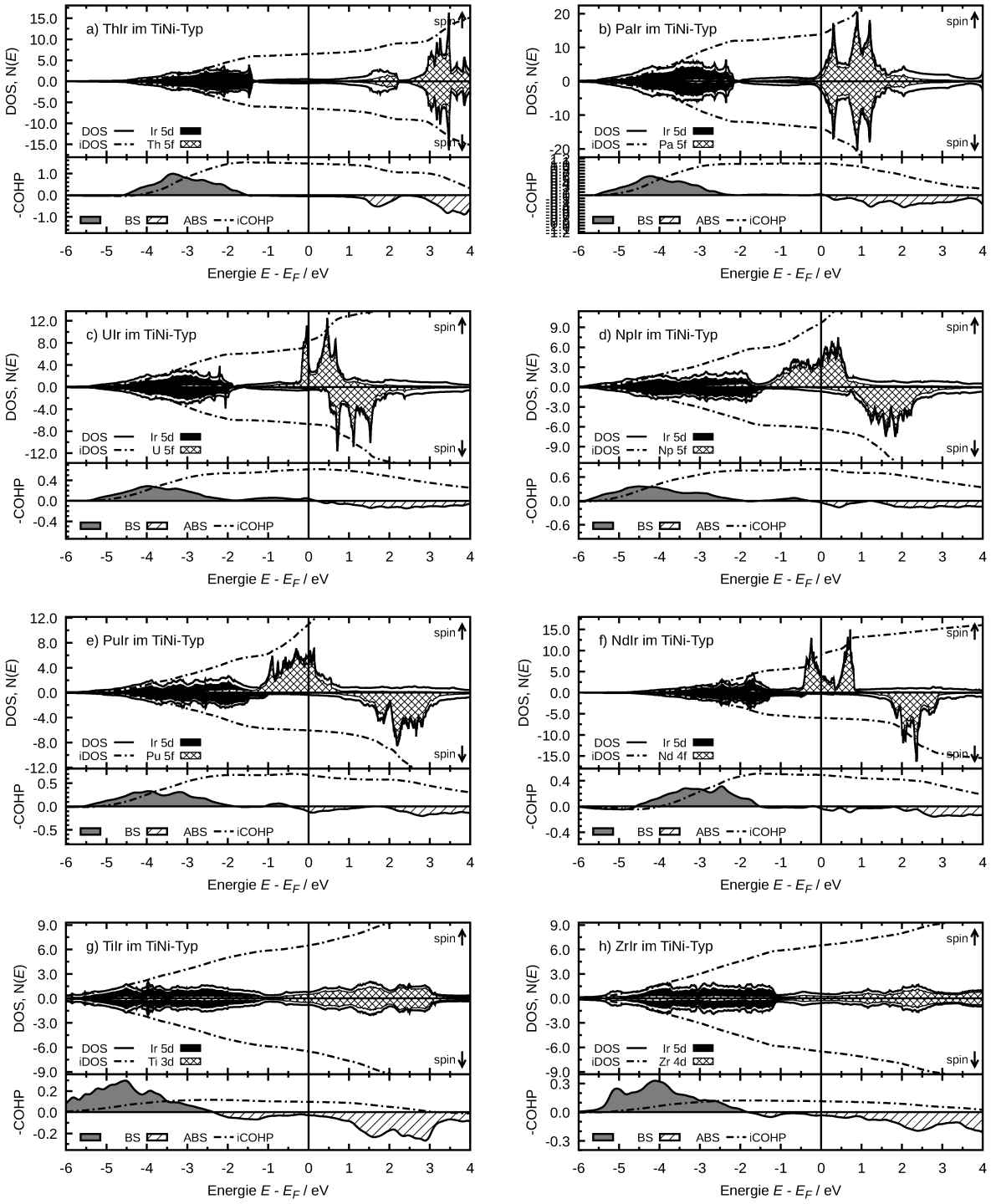

Abbildung A.3.15: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im TiNi-Typ für $N =$ Ir und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

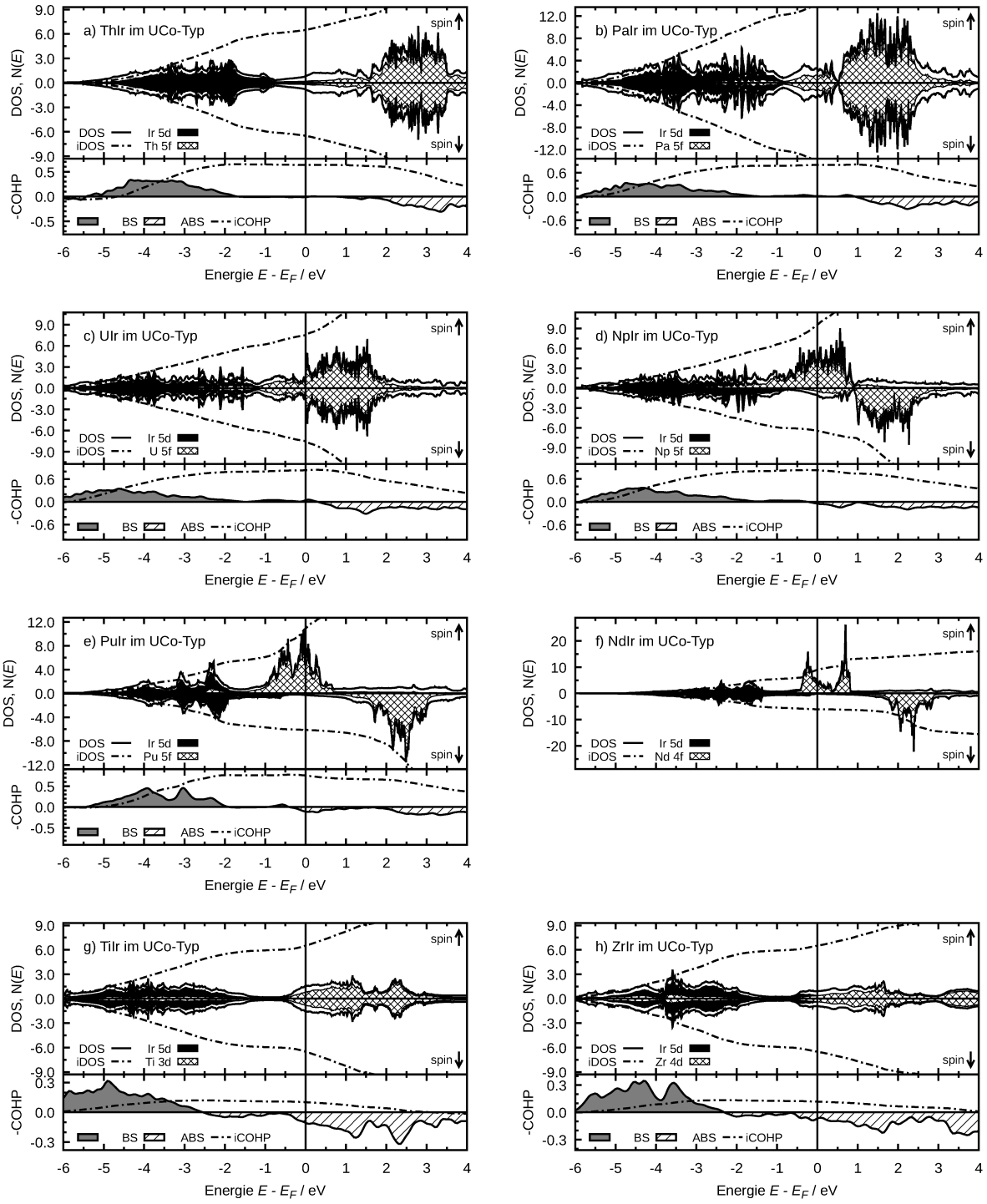

Abbildung A.3.16: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im UCo-Typ für $N =$ Ir und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

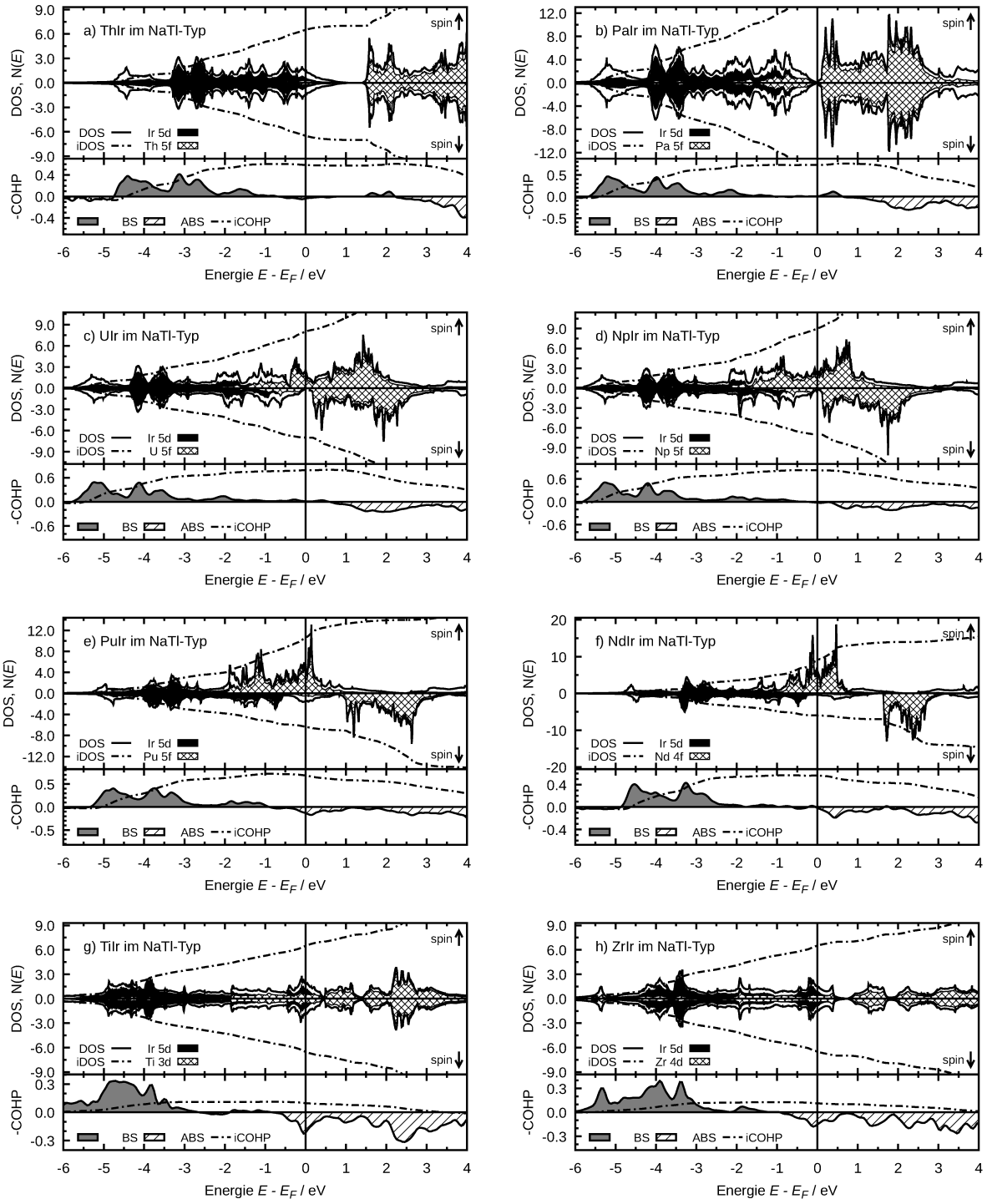

Abbildung A.3.17: DOS, pDOS und gemittelte COHP-Kurve der MN-Verbindungen im NaTl-Typ für $N =$ Ir und $M =$ **(a)** Th, **(b)** Pa, **(c)** U, **(d)** Np, **(e)** Pu, **(f)** Nd, **(g)** Ti und **(h)** Zr. PBE-Rechnungen mit Spinpolarisation und skalar-relativistischer PAW-Basis.

A.4 Anhang Kapitel 7: Zum Auftreten des NaTl-Strukturtyps

A.4.1 Strukturoptimierungen

Tabelle A.4.1: Raumgruppe, Pearson-Symbol, Gitterparameter, Kompressionsmodul K und Bildungsenthalpien ΔH_f pro Atom von UCo_x-Verbindungen. PAW-Rechnungen mit SOC und Spinpolarisation in der LDA-, PBE- und LDA+U-Näherung ($U = 1.5\,\mathrm{eV}$, $J = 0.5\,\mathrm{eV}$). Magnetische Achse entlang [001]. [Übernommen und überarbeitet mit Erlaubnis von M. Sachs, A. J. Karttunen, F. Kraus, *J. Phys.: Condens. Matter* **2019**, *31*, 025501. Copyright 2018 IOP Publishing.]

Verbindung	Raumgruppe, Pearson-Symbol	Methode	Gitterparameter / Å			K/ GPa	ΔH_f / kJ mol^{-1}	
			a	b	c		DFT	Miedema
Co (hcp)	$P6_3/mmc$, $hP2$	LDA	2.434	–	3.886	268	0	0
		LDA+U	2.434	–	3.886	268	0	0
		PBE	2.497	–	4.038	215	0	0
UCo_2	$Fd\bar{3}m$, $cF24$	LDA	6.840	–	–	230	−33	−31
		LDA+U	6.870	–	–	218	−36	−31
		PBE	7.004	–	–	188	−30	−31
UCo (UCo-Typ)	$I2_13$, $cI16$	LDA	6.265	–	–	222	−33	−33
		LDA+U	6.274	–	–	210	−36	−33
		PBE	6.317	–	–	188	−32	−33
U_6Co	$I4/mcm$, $tI28$	LDA	10.109	–	5.011	161	−5	−10
		LDA+U	10.145	–	5.173	153	−9	−10
		PBE	10.249	–	5.190	147	−10	−10
α-U	$Cmcm$, $oS4$	LDA	2.753	5.773	4.867	176	0	0
		LDA+U	2.802	5.820	4.893	148	0	0
		PBE	2.817	5.869	4.923	136	0	0

Tabelle A.4.2: Verwendete Atomradien für Nachbardiagramme aus PBE-Strukturoptimierungen der Elemente in bcc-Struktur. Skalar-relativistische PBE-PAW-Rechnungen mit Spinpolarisation.

Element	r/Å	Element	r/Å	Element	r/Å
Ti	1.408	Zr	1.547	Nd	1.722
Th	1.743	Pa	1.590	U	1.485
Np	1.421	Pu	1.450	Co	1.218
Rh	1.331	Ir	1.352		

A.5 Anhang Kapitel 8: Über die strukturelle Verzerrung im UCo-Strukturtyp und Kapitel 9: Über die strukturelle Verzerrung und Magnetismus von UIr

A.5.1 Details zur Phasenanalyse von UCo

Tabelle A.5.1: Massenanteil der Fremdphasen bei der Synthese von UCo.

Probe	Synthesebedingung	UCo		UCo_2		UO_x
		ω / %	a / Å	ω / %	a / Å	ω / %
MSa38		71	6.359	19	7.012	10
MSa42		74	6.359	18	7.012	8
BC44-temp2		84	6.360	12	7.013	4

A.5.2 Ergebnisse zur Einkristallstrukturanalyse von UIr

Tabelle A.5.2: Temperaturfaktoren U_{ij} / pm^2 von UIr aus der Einkristall-Strukturanalyse (Probe MSa78) und der Rietveld-Verfeinerung (Probe BC09). Alle Atome auf der Wyckoff-Position (4*e*). [Übernommen mit Erlaubnis von M. Sachs *et al.*, *Inorg. Chem.* **2021**, *60*, 16686–16699. Copyright 2021 American Chemical Society.]

Methode	Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Einkristall	U1	115(4)	88(3)	66(4)	0	10(2)	0	90(2)
	U2	111(4)	108(3)	79(4)	0	14(2)	0	99(2)
	Ir1	134(5)	94(3)	80(4)	0	31(3)	0	101(2)
	Ir2	123(4)	100(3)	94(4)	0	31(3)	0	104(2)
Rietveld	U1	132(18)	110(20)	132	0	0	0	127(12)
	U2	132	110	132	0	0	0	127
	Ir1	170(30)	60(30)	170	0	80(30)	0	127(16)
	Ir2	170	60	170	0	80	0	127

Tabelle A.5.3: Ausgewählte Atomabstände von UIr aus der Einkristall-Strukturanalyse (Probe MSa78) im Vergleich zur Literatur[5] und DFT-Rechnungen dieser Arbeit. Zur Vergleichbarkeit erfolgt die Benennung der Atome entsprechend der Aufspaltung der Wyckoff-Position 4*e* in zweimal 2*a* beim Übergang der Raumgruppe $P2_1/c$ in ihre Untergruppe $P2_1$. Die Atome U1 und $U1_1$ und alle anderen Paare besetzen dieselbe Lage 4*e* in der Aufstellung in Raumgruppe $P2_1/c$. [Übernommen mit Erlaubnis von M. Sachs *et al.*, *Inorg. Chem.* **2021**, *60*, 16686–16699. Copyright 2021 American Chemical Society.]

Atom 1	Atom 2	d/Å		
		Literatur	Diese Arbeit	DFT
U1	Ir1	2.82(1)	2.805(2)	2.792
	$Ir2_1$	2.84(2)	2.861(2)	2.848
	$Ir1_1$	2.85(2)	2.841(2)	2.827
	$Ir2_1$	2.85(2)	2.872(2)	2.864
	$Ir1_1$	2.87(2)	2.853(2)	2.845
	Ir2	3.12(2)	3.003(2)	3.062
	Ir1	3.17(1)	2.959(2)	2.980
	$U2_1$	3.41(2)	3.510(2)	3.554
	$U1_1$	3.53(2)	3.622(2)	3.671
	U2	3.634(9)	3.564(2)	3.567
	$U2_1$	3.65(2)	3.663(2)	3.624
	U2	3.67(2)	3.753(2)	3.772
	$U2_1$	3.68(2)	3.833(2)	3.872
	$U1_1$	3.74(1)	3.622(2)	3.672
	$U1_1$	3.77(2)	3.873(2)	3.840
	U2	3.83(2)	3.893(2)	3.897
$U1_1$	Ir11	2.80(1)	2.805	2.792
	Ir2	2.83(2)	2.861	2.848
	Ir1	2.84(2)	2.841	2.827
	Ir2	2.85(2)	2.872	2.864
	Ir1	2.87(2)	2.853	2.846
	$Ir1_1$	2.92(2)	2.959	2.980
	$Ir2_1$	3.01(1)	3.003	3.062
	$U2_1$	3.49(2)	3.510	3.554
	U2	3.59(2)	3.564	3.567
	U2	3.67(2)	3.753	3.624
	$U2_1$	3.80(3)	3.833	3.772
U2	Ir2	2.80(1)	2.824(2)	2.808
	$Ir1_1$	2.85(1)	2.862(2)	2.839
	$Ir2_1$	2.85(1)	2.831(2)	2.808
	$Ir1_1$	2.86(1)	2.865(2)	2.872
	$Ir2_1$	2.87(2)	2.848(2)	2.847
	Ir1	3.018(8)	3.158(1)	3.189
	Ir2	3.036(8)	3.253(2)	3.273
	$U2_1$	3.51(2)	3.399(2)	3.319
	$U2_1$	3.59(2)	3.665(2)	3.728
	$U2_1$	3.84(2)	3.665(2)	3.728

Atom 1	Atom 2	d/Å		
		Literatur	Diese Arbeit	DFT
$U2_1$	Ir1	2.80(3)	2.862	2.839
	Ir2	2.83(3)	2.824	2.808
	$Ir2_1$	2.82(2)	2.831	2.808
	Ir1	2.86(3)	2.865	2.872
	Ir2	2.87(3)	2.848	2.847
	$Ir1_1$	3.14(2)	3.158	3.189
	$Ir2_1$	3.28(2)	3.253	3.273
Ir1	$Ir2_1$	2.89(1)	2.953(2)	3.053
	$Ir1_1$	2.97(1)	2.981(2)	3.070
	Ir2	3.41(2)	3.221(2)	3.239
$Ir1_1$	Ir2	2.98(1)	2.953	3.053
	Ir21	3.173(8)	3.221	3.239
Ir2	$Ir2_1$	2.93(1)	2.908(2)	2.990

A.6 Anhang zu Kapitel 10: PAW-Basisfunktionen für die Actinoide

A.6.1 Input-Dateien für PAW-Basisfunktionen

Die Input-Dateien sind für die PAW-Datensätze des PBE-Funktionals angegeben. Für die LDA-PW-Datensätze muss `dft = 'pw'` gesetzt werden. USPP-Datensätze werden über `lpaw = 'false'` erzeugt. Die Datenstruktur ist im Online-Benutzerhandbuch erläutert.

A.6.1.1 Skalar-relativische PAW-Basisfunktionen

PAW-Basis für Th-Atome

```
&input
title = 'Thorium'
atom = 'Th',
dft = 'pbe',
config = '[Rn] 5f0.1 6d1.9 7s2 7p0',
rel = 1,
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Th.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.50
nlcc = .true.
new_core_ps=.true.
rcore = 1.2,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.80  0.0
7S  2  0  2.00  0.00  1.30  1.80  0.0
6P  2  1  6.00  0.00  1.60  2.00  0.0
7P  3  1  0.00  2.50  1.50  2.00  0.0
6D  3  2  1.90  0.00  1.60  2.20  0.0
6D  3  2  0.00  3.50  1.60  2.20  0.0
5F  4  3  0.10  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.50  1.30  2.20  0.0
```

PAW-Basis für Pa-Atome

```
&input
title = 'Protactinium'
atom = 'Pa',
dft = 'pbe',
config = '[Rn] 5f2.0 6d1.0 7s2 7p0',
rel = 1,
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Pa.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.5
nlcc = .true.
new_core_ps=.true.
rcore = 1.2,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.false.,
use_paw_as_gipaw=.false.,
/
8
6S  1  0  2.00  0.00  1.30  1.80  0.0
7S  2  0  2.00  0.00  1.30  1.80  0.0
6P  2  1  6.00  0.00  1.50  2.00  0.0
7P  3  1  0.00  2.50  1.40  2.00  0.0
6D  3  2  1.00  0.00  1.50  2.20  0.0
6D  3  2  0.00  3.50  1.50  2.20  0.0
5F  4  3  2.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.50  1.30  2.25  0.0
```

PAW-Basis für U-Atome

```
&input
title = 'Uran'
atom = 'U',
dft = 'pbe',
config = '[Rn] 5f3.0 6d1.0 7s2 7p0',
rel = 1,
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='U.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.4
nlcc = .true.
new_core_ps=.true.
rcore = 1.15,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.75  0.0
7S  2  0  2.00  0.00  1.30  1.75  0.0
6P  2  1  6.00  0.00  1.40  2.00  0.0
7P  3  1  0.00  3.50  1.40  2.00  0.0
6D  3  2  1.00  0.00  1.30  2.20  0.0
6D  3  2  0.00  3.50  1.30  2.20  0.0
5F  4  3  3.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.20  1.30  2.30  0.0
```

PAW-Basis für Np-Atome

```
&input
title = 'Neptunium'
atom = 'Np',
dft = 'pbe',
config = '[Rn] 5f4.0 6d1.0 7s2.0 7p0',
rel = 1,
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Np.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.3
nlcc = .true.
new_core_ps=.true.
rcore = 1.15,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.60  0.0
7S  2  0  2.00  0.00  1.30  1.60  0.0
6P  2  1  6.00  0.00  1.40  2.00  0.0
7P  3  1  0.00  3.50  1.40  2.00  0.0
6D  3  2  1.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  2.50  1.40  2.20  0.0
5F  4  3  4.00  0.00  1.40  1.80  0.0
5F  4  3  0.00  0.50  1.40  2.30  0.0
```

PAW-Basis für Pu-Atome

```
&input
title='Plutonium',
zed=94.0,
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0. 5f6.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Pu.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.3,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.1,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  2.00  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.40  2.00  0.0
7P  3  1  0.00  3.50  1.40  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3  6.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  0.95  1.30  2.30  0.0
```

PAW-Basis für Am-Atome

```
&input
title='Americium',
zed=95.0,
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f7.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Am.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.3,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.1,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.70  0.0
7S  2  0  2.00  0.00  1.30  1.70  0.0
6P  2  1  6.00  0.00  1.30  1.90  0.0
7P  3  1  0.00  1.50  1.30  1.90  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3  7.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.10  1.30  2.20  0.0
```

PAW-Basis für Cm-Atome

```
&input
title='Curium',
zed=96.0,
dft = 'pbe',
rel=1,
config='[Rn] 6d1.0 7s2.0 7p0.0 5f7.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Cm.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.30,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.65  0.0
7S  2  0  2.00  0.00  1.20  1.65  0.0
6P  2  1  6.00  0.00  1.30  1.90  0.0
7P  3  1  0.00  3.50  1.30  1.90  0.0
6D  3  2  1.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.50  1.40  2.10  0.0
5F  4  3  7.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  0.85  1.20  2.10  0.0
```

PAW-Basis für Bk-Atome

```
&input
title='Berkelium',
zed=97.0,
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f9.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Bk.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.30,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.65  0.0
7S  2  0  2.00  0.00  1.20  1.65  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3  9.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  1.10  1.20  2.10  0.0
```

PAW-Basis für Cf-Atome

```
&input
title='Californium',
atom='Cf'
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f10.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Cf.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.25,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  2.00  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  3.00  1.30  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3 10.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  1.00  1.20  2.00  0.0
```

PAW-Basis für Es-Atome

```
&input
title='Einsteinium',
atom='Es'
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f11.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Es.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.25,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.00,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  2.00  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  4.00  1.30  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3 11.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.10  1.20  1.95  0.0
```

PAW-Basis für Fm-Atome

```
&input
title = 'Fermium'
atom = 'Fm',
dft = 'pbe',
config = '[Rn] 5f12.0 6d0.0 7s2.0 7p0',
rel = 1,
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Fm.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.25
nlcc = .true.
new_core_ps=.true.
rcore = 1.0,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  2.00  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.30  1.90  0.0
7P  3  1  0.00  4.50  1.30  1.90  0.0
6D  3  2  0.00  0.00  1.40  2.00  0.0
6D  3  2  0.00  3.00  1.40  2.00  0.0
5F  4  3 12.00  0.00  1.30  1.90  0.0
5F  4  3  0.00  1.35  1.20  1.95  0.0
```

PAW-Basis für Md-Atome

```
&input
title='Mendelevium',
atom = 'Md'
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f13.0',
iswitch=3,
     /
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Md.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.20,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.15  1.60  0.0
7S  2  0  2.00  0.00  1.15  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  4.50  1.30  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.00  1.40  2.20  0.0
5F  4  3 13.00  0.00  1.25  1.80  0.0
5F  4  3  0.00  0.60  1.25  1.95  0.0
```

PAW-Basis für No-Atome

```
&input
title='Nobelium',
atom = 'No'
dft = 'pbe',
rel=1,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f14.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='No.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.20,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.10  1.55  0.0
7S  2  0  2.00  0.00  1.10  1.55  0.0
6P  2  1  6.00  0.00  1.20  2.00  0.0
7P  3  1  0.00  2.00  1.20  2.00  0.0
6D  3  2  0.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.00  1.40  2.10  0.0
5F  4  3 14.00  0.00  1.20  1.70  0.0
5F  4  3  0.00  1.50  1.20  1.90  0.0
```

PAW-Basis für Lr-Atome

```
&input
title='Lawrencium',
atom = 'Lr'
dft = 'pbe',
rel=1,
config='[Rn] 6d1.0 7s2.0 7p0.0 5f14.0',
iswitch=3,
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Lr.pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.15,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.10  1.50  0.0
7S  2  0  2.00  0.00  1.10  1.50  0.0
6P  2  1  6.00  0.00  1.20  2.00  0.0
7P  3  1  0.00  2.00  1.20  2.00  0.0
6D  3  2  1.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.00  1.40  2.10  0.0
5F  4  3 14.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  1.20  1.20  1.85  0.0
```

A.6.1.2 Voll-relativistische PAW-Basisfunktionen

PAW-Basis für U-Atome

```
&input
title = 'Uran'
atom = 'U',
dft = 'pbe',
config = '[Rn] 5f3.0 6d1.0 7s1.9 7p0',
rel = 2,
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='U.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.4
nlcc = .true.
new_core_ps=.true.
rcore = 1.15,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
file_core = 'core.dat'
/
9
6S  1  0  2.00  0.00  1.30  1.75  0.0
7S  2  0  1.90  0.00  1.30  1.75  0.0
6P  2  1  6.00  0.00  1.40  2.10  0.0
7P  3  1  0.00  0.50  1.40  2.10  0.5
7P  3  1  0.00  3.50  1.40  2.20  1.5
6D  3  2  1.00  0.00  1.30  2.20  0.0
6D  3  2  0.00  3.50  1.30  2.20  0.0
5F  4  3  3.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.20  1.30  2.30  0.0
```

PAW-Basis für Pa-Atome

```
&input
title = 'Protactinium'
atom = 'Pa',
dft = 'pbe',
config = '[Rn] 5f2.0 6d1.0 7s1.9 7p0',
rel = 2,
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Pa.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.5
nlcc = .true.
new_core_ps=.true.
rcore = 1.2,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.false.,
use_paw_as_gipaw=.false.,
/
8
6S  1  0  2.00  0.00  1.30  1.80  0.0
7S  2  0  1.90  0.00  1.30  1.80  0.0
6P  2  1  6.00  0.00  1.50  2.20  0.0
7P  3  1  0.00  2.50  1.40  2.20  0.0
6D  3  2  1.00  0.00  1.50  2.20  0.0
6D  3  2  0.00  3.50  1.50  2.20  0.0
5F  4  3  2.00  0.00  1.30  1.80  0.0
5F  4  3  0.00  1.50  1.30  2.25  0.0
```

PAW-Basis für Th-Atome

```
&input
title = 'Thorium'
atom = 'Th',
dft = 'pbe',
config = '[Rn] 5f0.0 6d2.0 7s1.9 7p0',
rel = 2,
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Th.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.50
nlcc = .true.
new_core_ps=.true.
rcore = 1.2,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.80  0.0
7S  2  0  1.90  0.00  1.30  1.80  0.0
6P  2  1  6.00  0.00  1.60  2.20  0.0
7P  3  1  0.00  2.50  1.50  2.20  0.0
6D  3  2  2.00  0.00  1.60  2.20  0.0
6D  3  2  0.00  3.50  1.60  2.20  0.0
5F  4  3  0.00  0.00  1.30  1.70  0.0
5F  4  3  0.00  1.50  1.30  2.20  0.0
```

PAW-Basis für Am-Atome

```
&input
title='Americium',
zed=95.0,
rel=2,
config='[Rn] 6d0.0 7s2.0 7p0.0 5f6.7',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Am.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.3,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.1,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.30  1.70  0.0
7S  2  0  2.00  0.00  1.30  1.70  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.5
7P  3  1  0.00  3.50  1.30  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.50  1.40  2.10  0.0
5F  4  3  6.70  0.00  1.30  1.80  0.0
5F  4  3  0.00  0.90  1.30  2.20  0.0
```

PAW-Basis für Pu-Atome

```
&input
title = 'Plutonium'
atom = 'Pu',
dft = 'pbe',
config = '[Rn] 5f6.0 6d0.0 7s1.6 7p0',
rel = 2,
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Pu.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.3
nlcc = .true.
new_core_ps=.true.
rcore = 1.1,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
10
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  1.60  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.40  2.00  0.0
7P  3  1  0.00  1.50  1.40  2.00  0.5
7P  3  1  0.00  3.50  1.40  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3  6.00  0.00  1.30  1.85  0.0
5F  4  3  0.00  0.95  1.30  2.20  2.5
5F  4  3  0.00  1.20  1.30  2.20  3.5
```

PAW-Basis für Np-Atome

```
&input
title = 'Neptunium'
atom = 'Np',
dft = 'pbe',
config = '[Rn] 5f4.0 6d1.0 7s1.9 7p0',
rel = 2,
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.
pseudotype=3,
file_pseudopw='Np.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc = -2,
rcloc = 1.3
nlcc = .true.
new_core_ps=.true.
rcore = 1.15,
which_augfun='PSQ',
rmatch_augfun_nc = .true.,
tm=.true.,
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
8
6S  1  0  2.00  0.00  1.30  1.55  0.0
7S  2  0  1.90  0.00  1.30  1.55  0.0
6P  2  1  6.00  0.00  1.40  2.10  0.0
7P  3  1  0.00  3.50  1.40  2.10  0.0
6D  3  2  1.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  2.50  1.40  2.20  0.0
5F  4  3  4.00  0.00  1.40  1.80  0.0
5F  4  3  0.00  0.50  1.40  2.30  0.0
```

PAW-Basis für Cf-Atome

```
&input
title='Californium',
atom='Cf'
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f10.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Cf.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.25,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.20  1.65  0.0
7S  2  0  1.40  0.00  1.20  1.65  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.5
7P  3  1  0.00  3.50  1.30  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3 10.00  0.00  1.30  1.75  0.0
5F  4  3  0.00  0.90  1.30  2.00  0.0
```

PAW-Basis für Bk-Atome

```
&input
title='Berkelium',
zed=97.0,
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f9.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Bk.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.30,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.20  1.65  0.0
7S  2  0  1.40  0.00  1.20  1.65  0.0
6P  2  1  6.00  0.00  1.30  1.90  0.0
7P  3  1  0.00  3.50  1.30  1.90  0.5
7P  3  1  0.00  4.00  1.30  2.00  1.5
6D  3  2  0.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  4.00  1.40  2.10  0.0
5F  4  3  9.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  1.10  1.20  2.05  0.0
```

PAW-Basis für Cm-Atome

```
&input
title='Curium',
zed=96.0,
rel=2,
config='[Rn] 6d1.0 7s1.6 7p0.0 5f7.0',
dft='pbe'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Cm.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.30,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.20  1.65  0.0
7S  2  0  1.60  0.00  1.20  1.65  0.0
6P  2  1  6.00  0.00  1.30  1.90  0.0
7P  3  1  0.00  2.50  1.30  1.90  0.5
7P  3  1  0.00  3.50  1.30  2.00  1.5
6D  3  2  1.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.50  1.40  2.10  0.0
5F  4  3  7.00  0.00  1.20  1.80  0.0
5F  4  3  0.00  0.85  1.20  2.10  0.0
```

PAW-Basis für Md-Atome

```
&input
title='Mendelevium',
atom='Md'
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f13.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Md.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.20,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
10
6S  1  0  2.00  0.00  1.15  1.60  0.0
7S  2  0  1.40  0.00  1.15  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.5
7P  3  1  0.00  4.00  1.30  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  4.00  1.40  2.10  0.0
5F  4  3 13.00  0.00  1.30  1.70  0.0
5F  4  3  0.00  0.80  1.15  1.95  2.5
5F  4  3  0.00  1.00  1.15  1.95  3.5
```

PAW-Basis für Fm-Atome

```
&input
title='Fermium',
atom='Fm'
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f12.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Fm.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.25,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.00,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
10
6S  1  0  2.00  0.00  1.15  1.60  0.0
7S  2  0  1.40  0.00  1.15  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.5
7P  3  1  0.00  4.00  1.30  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.00  0.0
6D  3  2  0.00  4.00  1.40  2.00  0.0
5F  4  3 12.00  0.00  1.30  1.75  0.0
5F  4  3  0.00  0.90  1.15  1.95  2.5
5F  4  3  0.00  1.00  1.15  1.95  3.5
```

PAW-Basis für Es-Atome

```
&input
title='Einsteinium',
atom='Es'
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f11.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Es.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.25,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=1.05,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.20  1.60  0.0
7S  2  0  1.40  0.00  1.20  1.60  0.0
6P  2  1  6.00  0.00  1.30  2.00  0.0
7P  3  1  0.00  2.50  1.30  2.00  0.5
7P  3  1  0.00  3.50  1.30  2.10  1.5
6D  3  2  0.00  0.00  1.40  2.20  0.0
6D  3  2  0.00  3.50  1.40  2.20  0.0
5F  4  3 11.00  0.00  1.30  1.75  0.0
5F  4  3  0.00  0.90  1.20  1.95  0.0
```

PAW-Basis für Lr-Atome

```
&input
title='Lawrencium',
atom='Lr'
rel=2,
config='[Rn] 6d0.0 7s2.0 7p0.4 5f14.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='Lr.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.20,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
9
6S  1  0  2.00  0.00  1.10  1.50  0.0
7S  2  0  2.00  0.00  1.10  1.50  0.0
6P  2  1  6.00  0.00  1.20  1.90  0.0
7P  3  1  0.40  0.00  1.20  1.90  0.5
7P  3  1  0.00  4.00  1.20  2.00  1.5
6D  3  2  0.00  0.00  1.30  1.90  0.0
6D  3  2  0.00  4.00  1.30  1.90  0.0
5F  4  3 14.00  0.00  1.20  1.90  0.0
5F  4  3  0.00  0.50  1.20  2.00 0.0
```

PAW-Basis für No-Atome

```
&input
title='Nobelium',
atom='No'
rel=2,
config='[Rn] 6d0.0 7s1.4 7p0.0 5f14.0',
dft='PBE'
dx = 0.008
iswitch = 3
/
&inputp
lpaw=.true.,
pseudotype=3,
file_pseudopw='No.rel-pbe-spn-kjpaw_MS.UPF',
author='Malte_Sachs',
lloc=-2,
rcloc=1.20,
which_augfun='PSQ',
rmatch_augfun_nc=.true.,
nlcc=.true.,
new_core_ps=.true.,
rcore=0.95,
tm=.true.
lgipaw_reconstruction=.true.,
use_paw_as_gipaw=.true.,
/
10
6S  1  0  2.00  0.00  1.10  1.55  0.0
7S  2  0  1.40  0.00  1.10  1.55  0.0
6P  2  1  6.00  0.00  1.20  1.90  0.0
7P  3  1  0.00  2.00  1.20  1.90  0.5
7P  3  1  0.00  4.00  1.20  2.00  1.5
6D  3  2  0.00  0.00  1.40  2.10  0.0
6D  3  2  0.00  3.00  1.40  2.10  0.0
5F  4  3 14.00  0.00  1.30  1.70  0.0
5F  4  3  0.00  0.75  1.20  1.95  2.5
5F  4  3  0.00  1.00  1.20  1.95  3.5
```

A.6.2 Input-Dateien für generierte LAPW+3LO-Basissätze

Folgende Input-Dateien können direkt mit dem LAPW-Programm *Elk* verwendet werden. Die Datenstruktur ist im Online-Benutzerhandbuch erläutert.

LAPW+3LO-Basis für Th-Atome

```
 'Th'
'thorium'
-90.0000
422979.5805
0.210819E-06    3.0   51.7499   800
26
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2   2.00000    F
7   0   1   2.00000    F
2
0.15   0  F
0.15   1  F
0
3
0   3
0.15      0  F
0.15      1  F
-1.6772   0  T
1   3
0.15      0  F
0.15      1  F
-0.7795   0  T
2   3
0.15   0  F
0.15   1  F
-3.2122   0  T
```

LAPW+3LO-Basis für Pa-Atome

```
 'Pa'
'protactinium'
-91.0000
421152.6452
0.209657E-06    2.82884361335   55.0947   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   2.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2  1.000000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
3
0   3
0.1500   0  F
0.1500   1  F
-1.6800   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8500   0  T
2   3
0.15     0  F
0.15     1  F
-3.4300   0  T
```

LAPW+3LO-Basis für U-Atome

```
 'U'
'uranium'
-92.0000
433900.1591
0.208514E-06    2.64757252629   55.1377   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   3.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2   1.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
3
0   3
0.1500   0  F
0.1500   1  F
-1.7600   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8600   0  T
2   3
0.1500   0  F
0.1500   1  F
-3.6400   0  T
```

LAPW+3LO-Basis für Np-Atome

```
 'Np'
'neptunium'
-93.0000
432024.5709
0.207390E-06    2.53014146006   55.1803   800
28
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   3.00000    F
5   3   4  1.000000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2  1.000000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
3
0   3
0.1500   0  F
0.1500   1  F
-1.8240   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8100   0  T
2   3
0.15     0  F
0.15     1  F
-3.72     0  T
```

LAPW+3LO-Basis für Pu-Atome

```
 'Pu'
'plutonium'
-94.0000
444784.7903
0.206284E-06    2.46508628367   58.7501   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   3.00000    F
5   3   4   3.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
3
0   3
0.1500   0  F
0.1500   1  F
-1.8100   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8300   0  T
2   3
0.1500   0  F
0.1500   1  F
-3.9000   0  T
```

LAPW+3LO-Basis für Am-Atome

```
 'Am'
'americium'
-95.0000
442961.9018
0.205196E-06    2.44022610408   51.9446   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   3.00000    F
5   3   4   4.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.0774   0  T
0   3
0.1500   0  F
0.1500   1  F
-1.8674   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.7549   0  T
2   3
0.1500   0  F
0.1500   1  F
-4.0900   0  T
```

LAPW+3LO-Basis für Cm-Atome

```
 'Cm'
'curium'
-96.0000
450253.4557
0.204124E-06    2.45500574777   55.3054   800
28
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   3.00000    F
5   3   4   4.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2  1.000000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.2184   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.0481   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8489   0  T
2   3
0.1500   0  F
0.1500   1  F
-4.4500   0  T
```

LAPW+3LO-Basis für Bk-Atome

```
 'Bk'
'berkelium'
-97.0000
450253.4557
0.203069E-06    2.49902950176   52.0199   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   5.00000    F
5   3   4   4.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.1057   0  T
0   3
0.1500   0  F
0.1500   1  F
-1.9965   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.7758   0  T
2   3
0.1500   0  F
0.1500   1  F
-4.4700   0  T
```

LAPW+3LO-Basis für Cf-Atome

```
 'Cf'
'californium'
-98.0000
457545.0097
0.202031E-06    2.58798803623   52.0569   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   4.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.1183   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.0620   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.7850   0  T
2   3
0.1500   0  F
0.1500   1  F
-4.6500   0  T
```

LAPW+3LO-Basis für Es-Atome

```
 'Es'
'einsteinium'
-99.0000
459367.8982
0.201008E-06    2.72173624788   48.9609   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   5.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.1339   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.1315   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.7952   0  T
2   3
0.1500   0  F
0.1500   1  F
-4.8400   0  T
```

LAPW+3LO-Basis für Fm-Atome

```
 'Fm'
'fermium'
-100.0000
468482.3406
0.200000E-06    2.8926585827   52.1300   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   6.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
0   3
0.1500   0  F
0.1500   1  F
-2.2021   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8046   0  T
2   3
0.1500   0  F
0.1500   1  F
-5.1000   0  T
3   3
0.1500   0  F
0.1500   1  F
-0.1000   0  T
```

LAPW+3LO-Basis für Md-Atome

```
 'Md'
'mendelevium'
-101.000
470305.2291
0.199007E-06    3.0   49.0271   800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   7.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.1623   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.2742   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8134   0  T
2   3
0.1500   0  F
0.1500   1  F
-5.2100   0  T
```

LAPW+3LO-Basis für No-Atome

```
 'No'
'nobelium'
-102.000
472128.1176
0.198030E-06    3.0   52.2018    800
27
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   8.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.1751   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.3481   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.8216   0  T
2   3
0.1500   0  F
0.1500   1  F
-5.3900   0  T
```

LAPW+3LO-Basis für Lr-Atome

```
 'Lr'
'lawrencium'
-103.000
477596.7830
0.197066E-06    3.0   65.5938    800
28
1   0   1   2.00000    T
2   0   1   2.00000    T
2   1   1   2.00000    T
2   1   2   4.00000    T
3   0   1   2.00000    T
3   1   1   2.00000    T
3   1   2   4.00000    T
3   2   2   4.00000    T
3   2   3   6.00000    T
4   0   1   2.00000    T
4   1   1   2.00000    T
4   1   2   4.00000    T
4   2   2   4.00000    T
4   2   3   6.00000    T
4   3   3   6.00000    T
4   3   4   8.00000    T
5   0   1   2.00000    T
5   1   1   2.00000    T
5   1   2   4.00000    T
5   2   2   4.00000    F
5   2   3   6.00000    F
5   3   3   6.00000    F
5   3   4   8.00000    F
6   0   1   2.00000    F
6   1   1   2.00000    F
6   1   2   4.00000    F
6   2   2  1.000000    F
7   0   1   2.00000    F
2
0.1500   0  F
0.1500   1  F
0
4
3   3
0.1500   0  F
0.1500   1  F
-0.3668   0  T
0   3
0.1500   0  F
0.1500   1  F
-2.5853   0  T
1   3
0.1500   0  F
0.1500   1  F
-0.9447   0  T
2   3
0.1500   0  F
0.1500   1  F
-5.8100   0  T
```

A.7 Literatur

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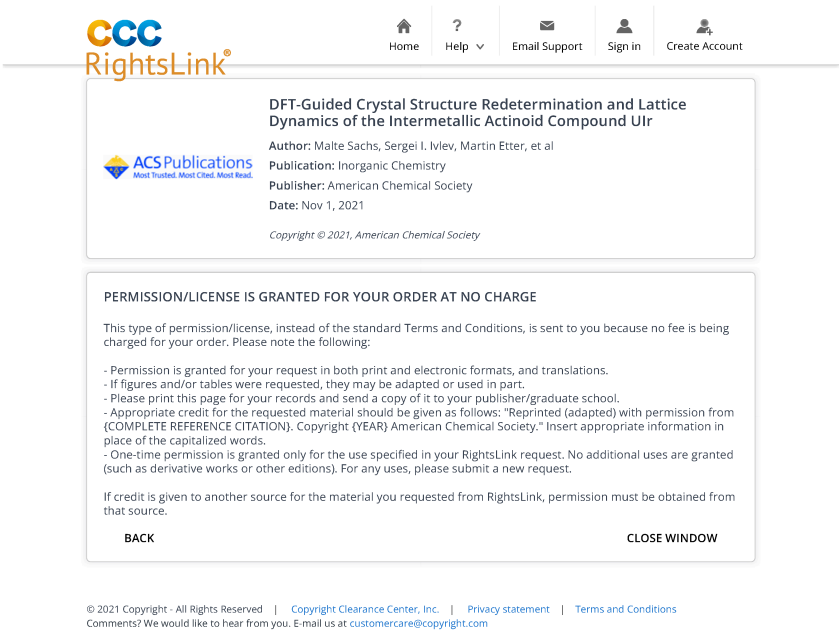

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