Supporting Information

Geometrical and electronic structure of Pt_7 cluster: A density functional study

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BPW91/LANL2DZ optimized geometries, Cartesian coordinates

Pt_2 triplet $D_{\infty h}$

Sum of electronic and zero-point Energies= -238.381074 Hartree

78	0.000000	0.000000	1.193181
78	0.000000	0.000000	-1.193181

Pt_7 singlet C_1 transition state

Sum of electronic and zero-point Energies= -834.619005 Hartree

78	0.000000	0.000000	1.182156
78	0.000000	1.463579	-1.033975
78	-2.191661	1.333268	0.221449
78	2.191661	1.333268	0.221449
78	0.000000	-1.463579	-1.033975
78	2.191661	-1.333268	0.221449
78	-2.191661	-1.333268	0.221449

Pt_7 triplet C_1 minimum

Sum of electronic and zero-point Energies= -834.675209 Hartree

78	2.055229	-1.303941	-0.305321
78	2.046504	1.309494	-0.306397
78	-0.006061	1.320563	1.269119
78	-2.051270	-1.298734	-0.304951
78	0.003570	-1.313393	1.271313
78	-2.056563	1.289200	-0.312864
78	0.008590	-0.003188	-1.310899

Pt_7 CTP quintet C_1 minimum

Sum of electronic and zero-point Energies= -834.670812 Hartree

78	-0.000311	-1.203699	1.150297
78	2.222359	-1.313977	-0.152227
78	-2.222899	-1.313427	-0.152600
78	0.000474	1.452327	1.195270
78	-2.032319	1.280214	-0.383490
78	2.032768	1.279653	-0.384001
78	-0.000071	-0.181090	-1.273250

Pt_7 CTP septet C_1 minimum

Sum of electronic and zero-point Energies= -834.678686 Hartree

78	2.218083	-1.334013	-0.137604
78	2.034955	1.260855	-0.410290
78	0.000231	1.503731	1.162439
78	-2.218933	-1.333338	-0.137093
78	0.000064	-1.139449	1.188435

78	-2.034142	1.261342	-0.410625
78	-0.000259	-0.219129	-1.255262

Pt_7 CTP multiplicity=9 C_1 minimum

Sum of electronic and zero-point Energies= -834.664443 Hartree

78	0.000733	-0.247308	-1.320836
78	-0.001037	1.382422	1.307483
78	1.939743	1.295647	-0.425690
78	-1.940607	1.294688	-0.426813
78	0.000415	-1.208477	1.192858
78	-2.218731	-1.259009	-0.163367
78	2.219484	-1.257962	-0.163635

Pt_7 CTP multiplicity =11 C_1 minimum

Sum of electronic and zero-point Energies= -834.617669 Hartree

78	0.000104	-0.000111	-1.205569
78	-0.000103	1.327622	1.149321
78	2.175822	1.307960	-0.273271
78	-2.175771	1.307938	-0.273629
78	-0.000103	-1.327419	1.149561
78	-2.175775	-1.307984	-0.273386
78	2.175826	-1.308006	-0.273026

Pt_7 CTP multiplicity =13 C_1 minimum

Sum of electronic and zero-point Energies= -834.558729 Hartree

78	0.000205	-0.000117	-1.306312
78	-0.000118	1.318387	1.041904
78	2.277688	1.275324	-0.194380
78	-2.277673	1.275324	-0.194724
78	-0.000118	-1.318195	1.042145
78	-2.277672	-1.275362	-0.194489
78	2.277688	-1.275362	-0.194145

Pt_7 ECTB singlet C_s minimum

Sum of electronic and zero-point Energies= -834.659169 Hartree

78	1.576979	-0.656221	0.000000
78	-0.108400	-2.749260	0.000000
78	-0.257843	1.613145	2.530890
78	-0.257843	1.613145	-2.530890
78	0.000000	1.562248	0.000000
78	-0.476446	-0.691528	-1.541117
78	-0.476446	-0.691528	1.541117

Pt_7 ECTB triplet C_s minimum

Sum of electronic and zero-point Energies= -834.673091 Hartree

78	1.637912	-0.590911	0.000000
78	0.157820	-2.795321	0.000000
78	-0.419704	1.602174	2.463447
78	-0.419704	1.602174	-2.463447
78	0.000000	1.648937	0.000000
78	-0.478162	-0.733526	-1.465790

78	-0.478162	-0.733526	1.465790

Pt_7 ECTB quintet C_s transition state

Sum of electronic and zero-point Energies= -834.667707 Hartree

78	1.689312	-0.481291	0.000000
78	0.357664	-2.765520	0.000000
78	-0.506704	1.555139	2.478586
78	-0.506704	1.555139	-2.478586
78	0.000000	1.648713	0.000000
78	-0.516784	-0.756090	-1.426117
78	-0.516784	-0.756090	1.426117

Pt_7 FCTB singlet C_1 minimum

Sum of electronic and zero-point Energies= -834.660070 Hartree

78	-0.117597	-0.523353	-1.275143
78	1.345517	-1.489017	0.741577
78	1.172952	1.258222	0.926358
78	-0.963634	-0.359223	1.472980
78	-1.205473	1.616027	-0.246811
78	-2.624444	-0.651914	-0.550358
78	2.392679	0.149257	-1.068603

Pt_7 FCTB triplet C_1 minimum

Sum of electronic and zero-point Energies= -834.667844 Hartree

78	-0.051112	-0.431137	-1.316341
78	1.355817	-1.537585	0.633435
78	1.057247	1.283186	0.974243
78	-0.943938	-0.483058	1.469695
78	-1.310433	1.609214	-0.193306
78	-2.563226	-0.685572	-0.603252
78	2.455645	0.244953	-0.964474

Pt_7 FCTB quintet C_1 minimum

Sum of electronic and zero-point Energies= -834.668201 Hartree

78	-0.002396	-0.000206	1.322380
78	1.559521	1.522945	-0.383015
78	0.922606	-1.054298	-1.144963
78	-0.919469	1.056000	-1.142428
78	-1.555869	-1.522914	-0.385170
78	-2.528138	0.553656	0.864431
78	2.523744	-0.555182	0.868765

Pt_7 ECT triplet C_s transistuin state

Sum of electronic and zero-point Energies= -834.667341 Hartree

78	1.723995	-0.265114	0.000000
78	-1.019402	-2.754013	0.000000
78	0.035140	1.451953	2.535109
78	0.035140	1.451953	-2.535109
78	0.000000	1.681961	0.000000
78	-0.387437	-0.783370	-1.451576
78	-0.387437	-0.783370	1.451576

Pt_7 ECT quintet C_s second order saddle point

Sum of electronic and zero-point Energies= -834.664126 Hartree

78	1.664495	-0.257439	0.000000
78	-1.226732	-2.706387	0.000000
78	0.272196	1.408509	2.528211
78	0.272196	1.408509	-2.528211
78	0.000000	1.656792	0.000000
78	-0.491077	-0.754992	-1.434579
78	-0.491077	-0.754992	1.434579

Pt_7 COh triplet C_3 minimum

Sum of electronic and zero-point Energies= -834.664944 Hartree

78	0.000000	0.000000	2.890938
78	0.000000	1.509597	0.683206
78	1.307350	-0.754799	0.683206
78	-1.307350	-0.754799	0.683206
78	-0.000089	-1.527690	-1.646852
78	-1.322974	0.763922	-1.646852
78	1.323063	0.763768	-1.646852

Pt_7 COh quintet C_1 minumum

Sum of electronic and zero-point Energies= -834.666217 Hartree

78	-2.871009	0.000403	0.000116
78	-0.655384	-1.485567	0.317640
78	-0.654757	0.467520	-1.445043
78	-0.654789	1.017960	1.127161
78	1.612260	1.512943	-0.323350
78	1.611971	-0.476393	1.471379
78	1.611708	-1.036865	-1.147904

Pt_7 COh septet C_1 transition state

Sum of electronic and zero-point Energies= -834.665455 Hartree

78	-2.786540	-0.003424	-0.001047
78	-0.601671	-0.881070	-1.304704
78	-0.699930	1.559614	0.015288
78	-0.604309	-0.915389	1.282272
78	1.478506	0.833668	1.360886
78	1.727548	-1.458694	-0.015640
78	1.486395	0.865294	-1.337056

Pt_7 TCT singlet C_s transition state

Sum of electronic and zero-point Energies= -834.646937 Hartree

78	0.000000	1.392854	0.000000
78	2.308680	0.110354	0.000000
78	-0.808156	0.729598	2.391932
78	-0.808156	0.729598	-2.391932
78	-1.708062	-0.510691	0.000000
78	0.507847	-1.225856	-1.393879
78	0.507847	-1.225856	1.393879

Pt_7 TCT triplet C_1 minimum

Sum of electronic and zero-point Energies= -834.659346 Hartree

78	0.040888	-0.001585	1.644151
78	2.400241	-0.012730	0.469786
78	-1.150754	-2.015270	0.535452
78	-1.127519	2.026808	0.537559
78	-1.737135	0.010110	-1.004656
78	0.794734	1.322239	-1.091036
78	0.779546	-1.329571	-1.091258

Pt_7 PBP singlet C_{2v} third order saddle point

Sum of electronic and zero-point Energies= -834.635189 Hartree

78	1.475042	0.000000	0.069818
78	0.000000	0.000000	2.279804
78	-1.475042	0.000000	0.069818
78	0.000000	2.164700	0.674316
78	0.000000	-2.164700	0.674316
78	0.000000	1.345020	-1.884036
78	0.000000	-1.345020	-1.884036

Pt_7 PBP triplet C_{2v} third order saddle point

Sum of electronic and zero-point Energies= -834.646563 Hartree

78	1.500186	0.000000	0.021933
78	0.000000	0.000000	2.255907
78	-1.500186	0.000000	0.021933
78	0.000000	2.194584	0.675323
78	0.000000	-2.194584	0.675323
78	0.000000	1.339214	-1.825209
78	0.000000	-1.339214	-1.825209

Pt_7 PBP quintet C_{2v} transition state

Sum of electronic and zero-point Energies= -834.651809 Hartree

78	1.436473	0.000000	0.062326
78	0.000000	0.000000	2.261788
78	-1.436473	0.000000	0.062326
78	0.000000	2.246462	0.651233
78	0.000000	-2.246462	0.651233
78	0.000000	1.354280	-1.844453
78	0.000000	-1.354280	-1.844453

Pt_7 PBP septet C_{2v} transition state

Sum of electronic and zero-point Energies= -834.650156 Hartree

78	1.457259	0.000000	-0.014474
78	0.000000	0.000000	2.159814
78	-1.457259	0.000000	-0.014474
78	0.000000	2.278188	0.713635
78	0.000000	-2.278188	0.713635
78	0.000000	1.447061	-1.779068
78	0.000000	-1.447061	-1.779068

Pt_7 ECR triplet C_s second order saddle point

Sum of electronic and zero-point Energies= -834.640807 Hartree

78	0.000000	1.083561	0.000000
78	0.816223	-1.485013	0.000000
78	2.544566	0.369375	0.000000
78	-1.849841	-0.956378	0.000000
78	1.851018	2.831010	0.000000
78	-2.480137	1.478483	0.000000
78	-0.881829	-3.321040	0.000000

Pt_7 ECR quintet C_s second order saddle point

Sum of electronic and zero-point Energies= -834.633060 Hartree

78	0.000000	1.033720	0.000000
78	0.804617	-1.496553	0.000000
78	2.601916	0.391705	0.000000
78	-1.832609	-0.925899	0.000000
78	1.831588	2.808876	0.000000
78	-2.484027	1.540780	0.000000
78	-0.921485	-3.352630	0.000000

Pt_7 W singlet C_{2v} third order saddle point

Sum of electronic and zero-point Energies= -834.588019 Hartree

78	0.000000	0.000000	1.216091
78	0.000000	1.337215	-1.042527
78	0.000000	-1.337215	-1.042527
78	0.000000	2.560110	1.303868
78	0.000000	-2.560110	1.303868
78	0.000000	3.923918	-0.869386
78	0.000000	-3.923918	-0.869386

Pt_7 W triplet C_{2v} third order saddle point

Sum of electronic and zero-point Energies= -834.604453 Hartree

78	0.000000	0.000000	1.278941
78	0.000000	1.287509	-1.015907
78	0.000000	-1.287509	-1.015907
78	0.000000	2.569233	1.314418
78	0.000000	-2.569233	1.314418
78	0.000000	3.853202	-0.937982
78	0.000000	-3.853202	-0.937982

Pt_7 W quintet C_{2v} fourth order saddle point

Sum of electronic and zero-point Energies= -834.594406 Hartree

78	0.000000	0.000000	1.227120
78	0.000000	1.356450	-1.024278
78	0.000000	-1.356450	-1.024278
78	0.000000	2.593931	1.328112
78	0.000000	-2.593931	1.328112
78	0.000000	3.910339	-0.917394
78	0.000000	-3.910339	-0.917394

Pt_7 ECP singlet C_{2v} third order saddle point

Sum of electronic and zero-point Energies= -834.554453 Hartree

78	0.000000	0.000000	1.743438
78	-1.430443	1.428134	0.037862
78	1.430443	1.428134	0.037862
78	1.430443	-1.428134	0.037862
78	-1.430443	-1.428134	0.037862
78	0.000000	3.293797	-0.947443
78	0.000000	-3.293797	-0.947443

Pt_7 ECP triplet C_{2v} fourth order saddle point

Sum of electronic and zero-point Energies= -834.601364 Hartree

78	0.000000	0.000000	1.802251
78	-1.419224	1.365710	0.052735
78	1.419224	1.365710	0.052735
78	1.419224	-1.365710	0.052735
78	-1.419224	-1.365710	0.052735
78	0.000000	3.207905	-1.006596
78	0.000000	-3.207905	-1.006596

Pt_7 ECP quintet C_{2v} second order saddle point

Sum of electronic and zero-point Energies= -834.600015 Hartree

78	0.000000	0.000000	1.811656
78	-1.312741	1.410817	-0.027937
78	1.312741	1.410817	-0.027937
78	1.312741	-1.410817	-0.027937
78	-1.312741	-1.410817	-0.027937
78	0.000000	3.473328	-0.849954
78	0.000000	-3.473328	-0.849954

Pt_7 ECS singlet C_{2v} transition state

Sum of electronic and zero-point Energies= -834.574148 Hartree

78	0.000000	0.000000	2.871794
78	0.000000	1.379140	0.762804
78	0.000000	-1.379140	0.762804
78	0.000000	3.627993	-0.428126
78	0.000000	-3.627993	-0.428126
78	0.000000	1.407759	-1.770576
78	0.000000	-1.407759	-1.770576

Pt_7 ECS triplet C_{2v} transition state

Sum of electronic and zero-point Energies= -834.595071 Hartree

78	0.000000	0.000000	2.936114
78	0.000000	1.349268	0.807196
78	0.000000	-1.349268	0.807196
78	0.000000	3.561930	-0.497075
78	0.000000	-3.561930	-0.497075
78	0.000000	1.362312	-1.778179
78	0.000000	-1.362312	-1.778179

Pt_7 ECS quintet C_{2v} second order saddle point

Sum of electronic and zero-point Energies= -834.581624 Hartree

78	0.000000	0.000000	2.903941

78	0.000000	1.440500	0.858624
78	0.000000	-1.440500	0.858624
78	0.000000	3.570445	-0.520861
78	0.000000	-3.570445	-0.520861
78	0.000000	1.352007	-1.789733
78	0.000000	-1.352007	-1.789733

Pt_7 HEX singlet D_{2h} second order saddle point

Sum of electronic and zero-point Energies= -834.586911 Hartree

78	0.000000	0.000000	0.000000
78	0.000000	0.000000	2.575288
78	0.000000	0.000000	-2.575288
78	0.000000	2.265101	1.482113
78	0.000000	-2.265101	1.482113
78	0.000000	-2.265101	-1.482113
78	0.000000	2.265101	-1.482113

Pt_7 HEX triplet D_{2h} fifth order saddle point

Sum of electronic and zero-point Energies= -834.576274 Hartree

78	0.000000	0.000000	0.000000
78	0.000000	0.000000	2.684660
78	0.000000	0.000000	-2.684660
78	0.000000	2.233527	1.444916
78	0.000000	-2.233527	1.444916
78	0.000000	-2.233527	-1.444916
78	0.000000	2.233527	-1.444916

Au_2 singlet $D_{\infty h}$ minimum

Sum of electronic and zero-point Energies= -271.062546 Hartree

79	0.000000	0.000000	1.275500
79	0.000000	0.000000	-1.275500

Au_7 ECR doublet C_s minimum

Sum of electronic and zero-point Energies= -948.877212 Hartree

79	-2.658027	1.577456	0.000000
79	-1.824264	-0.961072	0.000000
79	0.000000	1.155226	0.000000
79	-1.036913	-3.529968	0.000000
79	2.645886	0.388003	0.000000
79	0.926093	-1.676128	0.000000
79	1.947225	3.046482	0.000000

Au_7 ECS doublet C_{2v} transition state

Sum of electronic and zero-point Energies= -948.873995 Hartree

79	0.000000	0.000000	3.144519
79	0.000000	1.406437	0.872350
79	0.000000	-1.406437	0.872350
79	0.000000	3.704438	-0.556233
79	0.000000	-3.704438	-0.556233
79	0.000000	1.344438	-1.888376
79	0.000000	-1.344438	-1.888376

Au_7 ECT doublet C_{3v} minimum

Sum of electronic and zero-point Energies= -948.867451 Hartree

79	0.000000	0.000000	2.029285
79	0.000000	1.680339	-0.274896
79	1.455216	-0.840169	-0.274896
79	-1.455216	-0.840169	-0.274896
79	0.000000	-3.099054	-0.401533
79	-2.683860	1.549527	-0.401533
79	2.683860	1.549527	-0.401533

Au_7 HEX doublet D_{2h} minimum

Sum of electronic and zero-point Energies= -948.864290 Hartree

79	0.000000	0.000000	0.000000
79	0.000000	0.000000	2.718167
79	0.000000	0.000000	-2.718167
79	0.000000	2.413061	1.431877
79	0.000000	-2.413061	1.431877
79	0.000000	-2.413061	-1.431877
79	0.000000	2.413061	-1.431877

Au_7 TCT doublet C_{3v} minimum

Sum of electronic and zero-point Energies= -948.859684 Hartree

79	0.000000	0.000000	1.459126
79	0.000000	2.679350	0.494179
79	2.320385	-1.339675	0.494179
79	-2.320385	-1.339675	0.494179
79	0.000000	-1.656195	-0.980554
79	-1.434307	0.828097	-0.980554
79	1.434307	0.828097	-0.980554

Au_7 PBP doublet D_{5h} minimum

Sum of electronic and zero-point Energies= -948.858368 Hartree

79	0.000000	0.000000	1.553878
79	0.000000	2.395419	0.000000
79	0.000000	0.000000	-1.553878
79	2.278179	0.740225	0.000000
79	-2.278179	0.740225	0.000000
79	1.407992	-1.937935	0.000000
79	-1.407992	-1.937935	0.000000

Au_7 COh doublet C_s transition state

Sum of electronic and zero-point Energies= -948.853513 Hartree

79	-2.620039	1.048538	0.000000
79	0.000000	1.920122	0.000000
79	-0.913679	-0.656742	1.400127
79	-0.913679	-0.656742	-1.400127
79	0.897234	-2.222753	0.000000
79	1.775081	0.283789	-1.378759
79	1.775081	0.283789	1.378759

Au_7 ECP doublet C_{2v} transition state

Sum of electronic and zero-point Energies= -948.851983 Hartree

79	0.000000	0.000000	2.102901
79	-1.394730	1.387163	0.068561
79	1.394730	1.387163	0.068561
79	-1.394730	-1.387163	0.068561
79	1.394730	-1.387163	0.068561
79	0.000000	3.358898	-1.188572
79	0.000000	-3.358898	-1.188572

Au_7 W doublet C_{2v} minimum

Sum of electronic and zero-point Energies= -948.851414 Hartree

79	0.000000	0.000000	1.432532
79	0.000000	1.337378	-1.077107
79	0.000000	-1.337378	-1.077107
79	0.000000	2.735547	1.342190
79	0.000000	-2.735547	1.342190
79	0.000000	4.084624	-0.981349
79	0.000000	-4.084624	-0.981349

Au_7 CP doublet C_{2v} second order saddle point

Sum of electronic and zero-point Energies= -948.850272 Hartree

79	0.000000	0.000000	2.430851
79	-1.389741	1.412507	0.390543
79	1.389741	1.412507	0.390543
79	1.389741	-1.412507	0.390543
79	-1.389741	-1.412507	0.390543
79	0.000000	1.400399	-1.996511
79	0.000000	-1.400399	-1.996511

Au_7 CTP doublet C_{2v} second order saddle point

Sum of electronic and zero-point Energies= -948.846819 Hartree

79	0.000000	0.000000	1.205565
79	0.000000	1.450297	-1.352262
79	-2.182570	1.415122	0.374740
79	2.182570	1.415122	0.374740
79	0.000000	-1.450297	-1.352262
79	2.182570	-1.415122	0.374740
79	-2.182570	-1.415122	0.374740

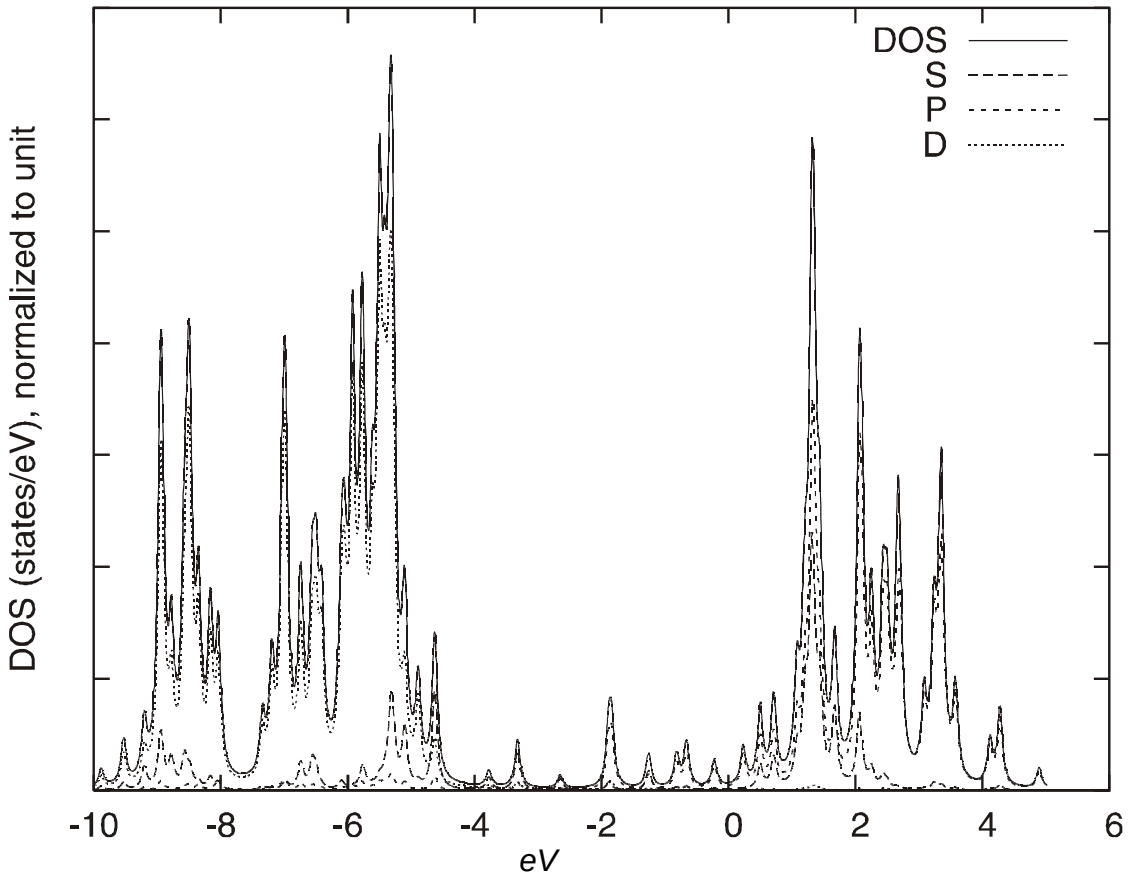

Figure 3aAS The alpha−spin density of states of quintet CTP Pt_7 cluster. DOS is the total alpha−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

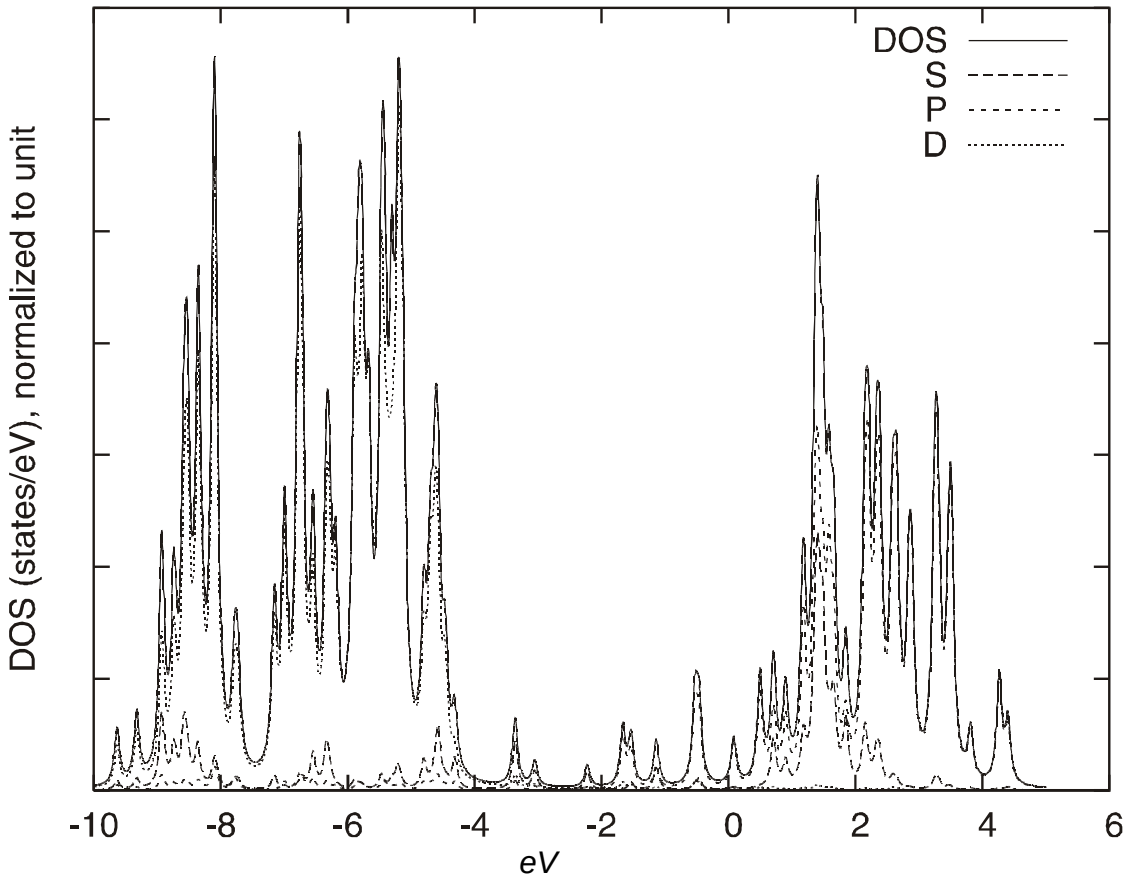

Figure 3aBS The beta–spin density of states of quintet CTP Pt_7 cluster. DOS is the total beta–spin density of states. S, P and D are the partial alpha–spin density of states for angular momentum *s*, *p* and *d*.

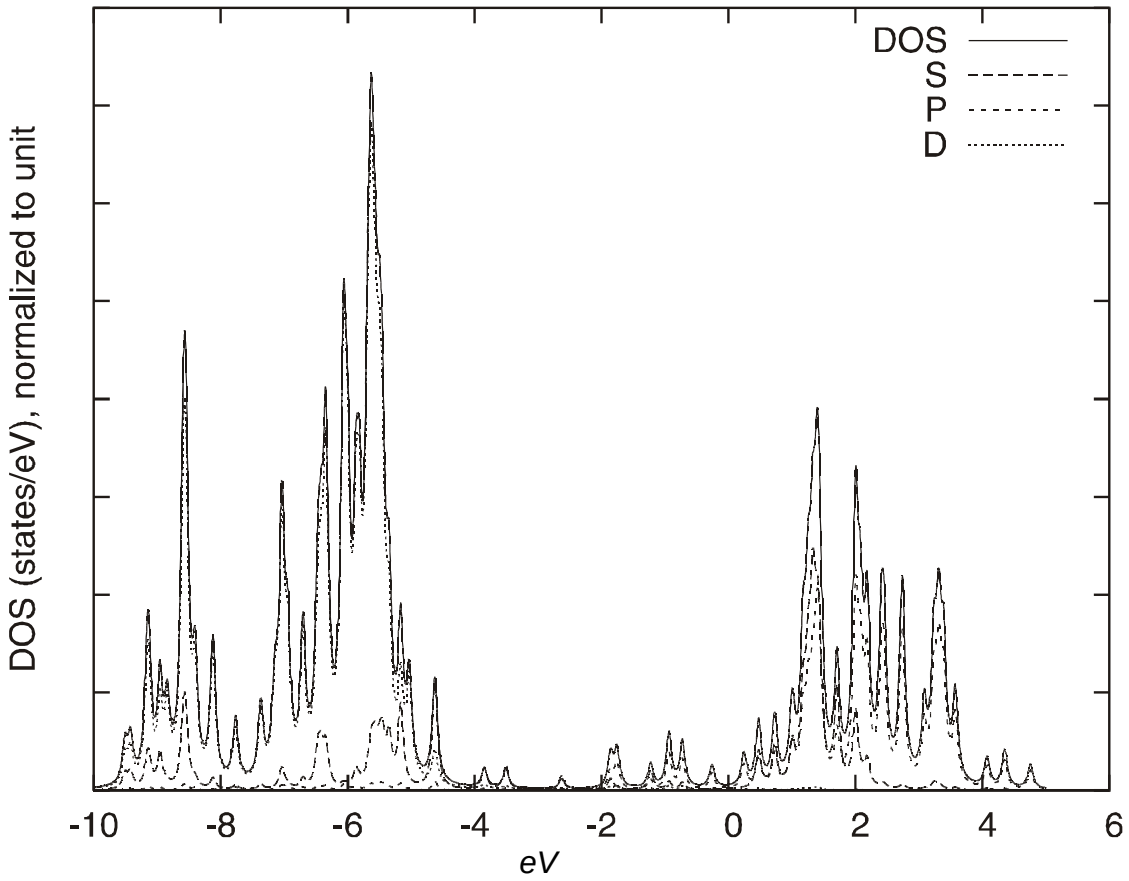

Figure 3bAS The alpha−spin density of states of septet CTP Pt_7 cluster. DOS is the total alpha−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

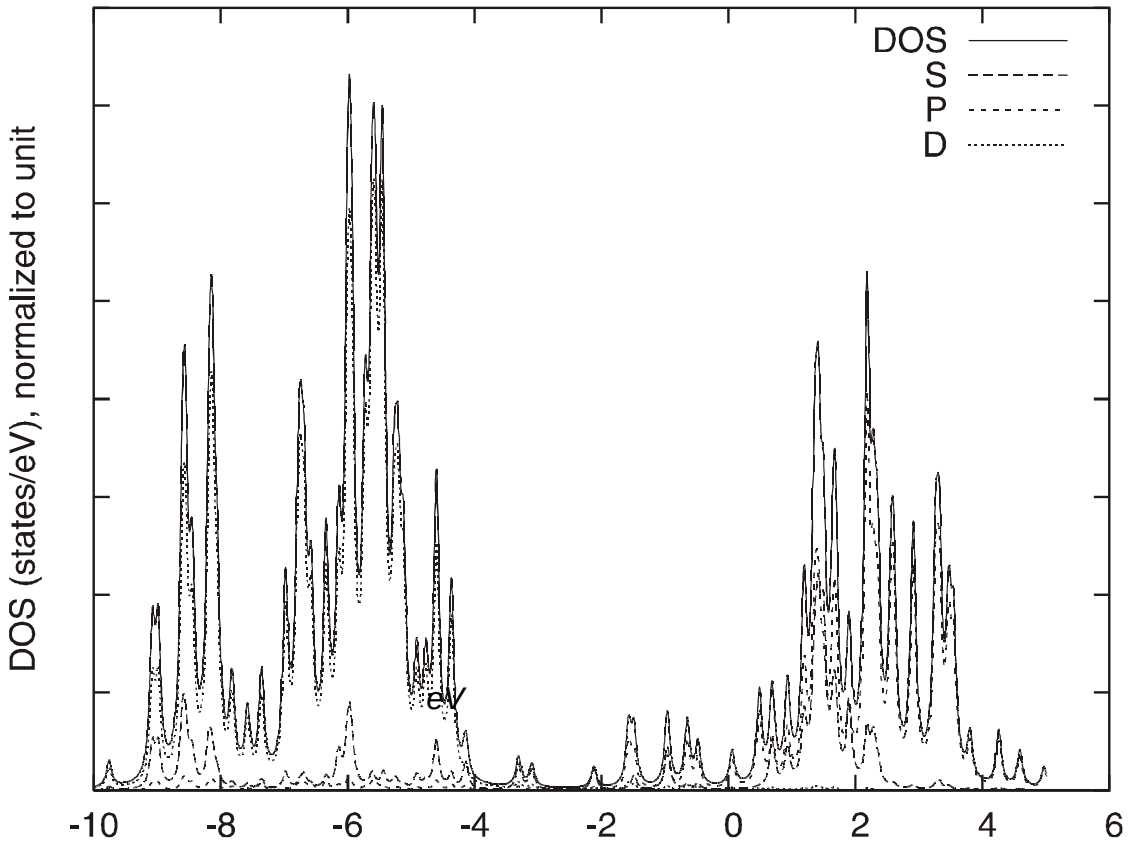

Figure 3bBS The beta−spin density of states of septet CTP Pt_7 cluster. DOS is the total beta−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

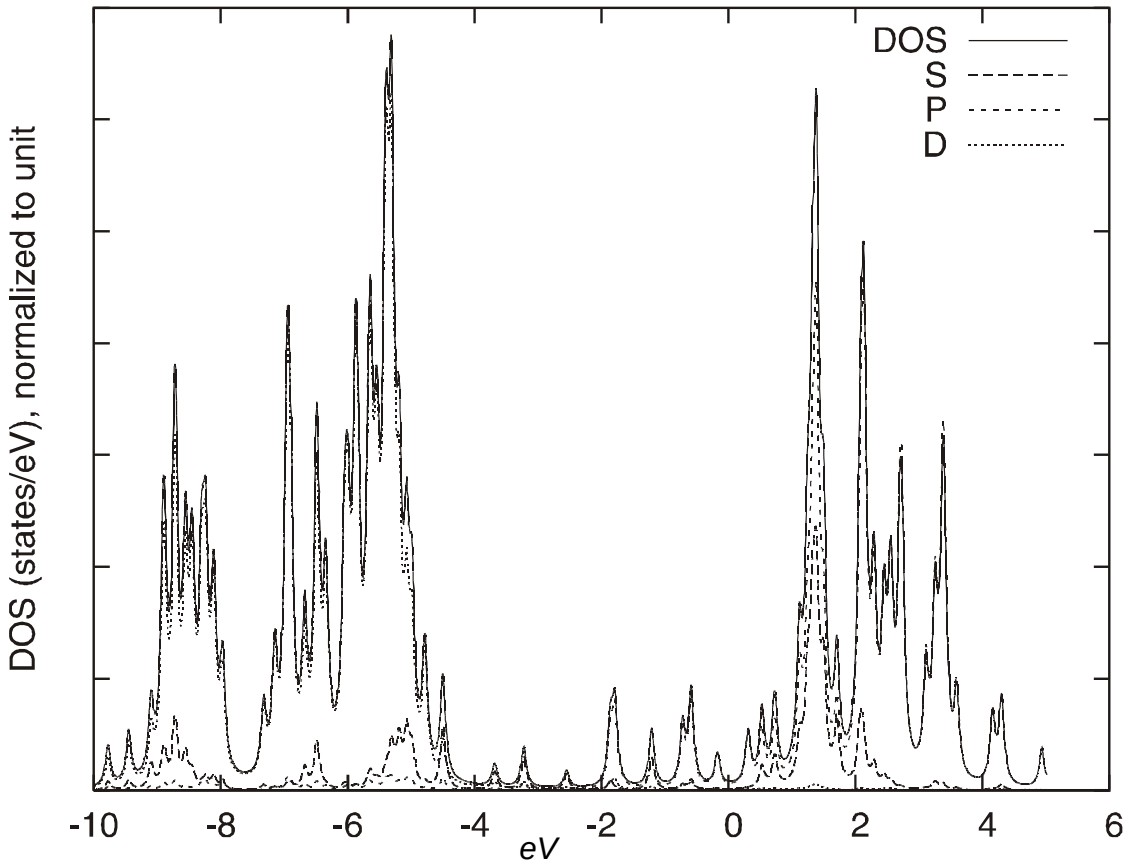

Figure 3cAS The alpha–spin density of states of triplet CTP Pt_7 cluster. DOS is the total alpha–spin density of states. S, P and D are the partial alpha–spin density of states for angular momentum *s*, *p* and *d*.

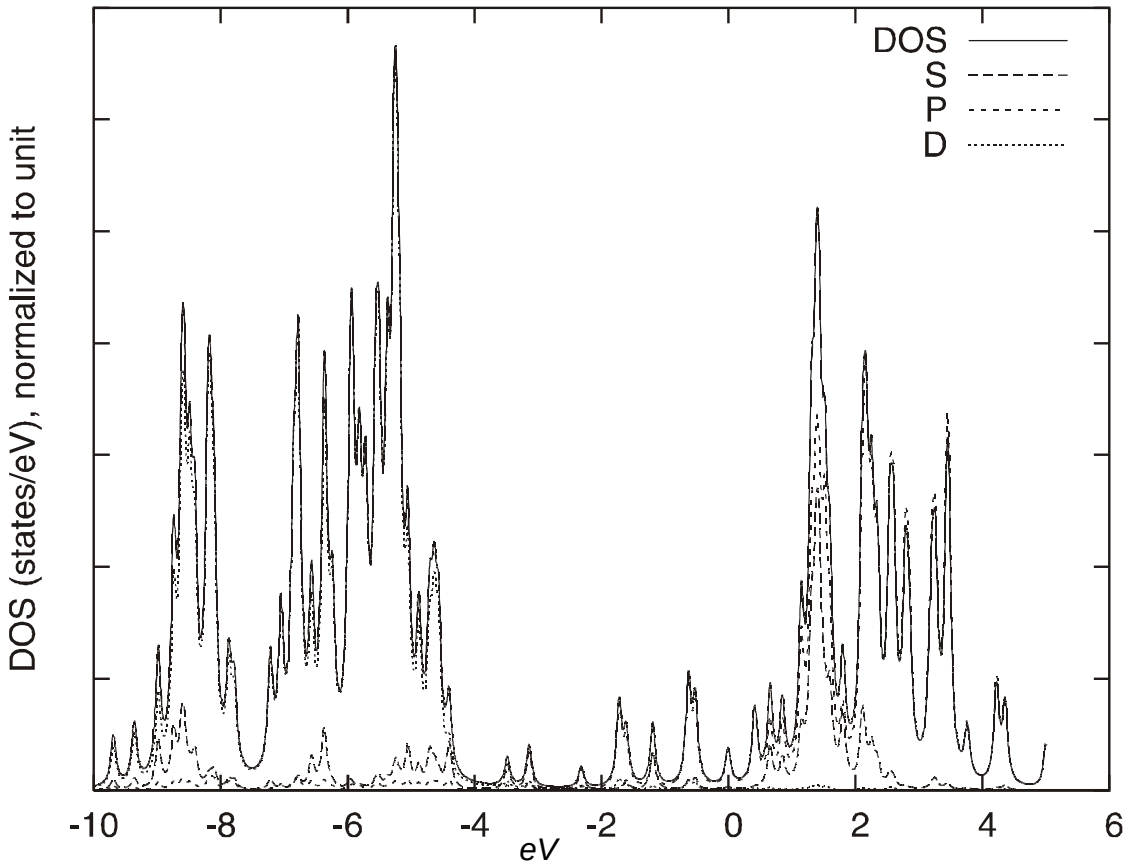

Figure 3cBS The beta–spin density of states of triplet CTP Pt_7 cluster. DOS is the total beta–spin density of states. S, P and D are the partial alpha–spin density of states for angular momentum *s*, *p* and *d*.

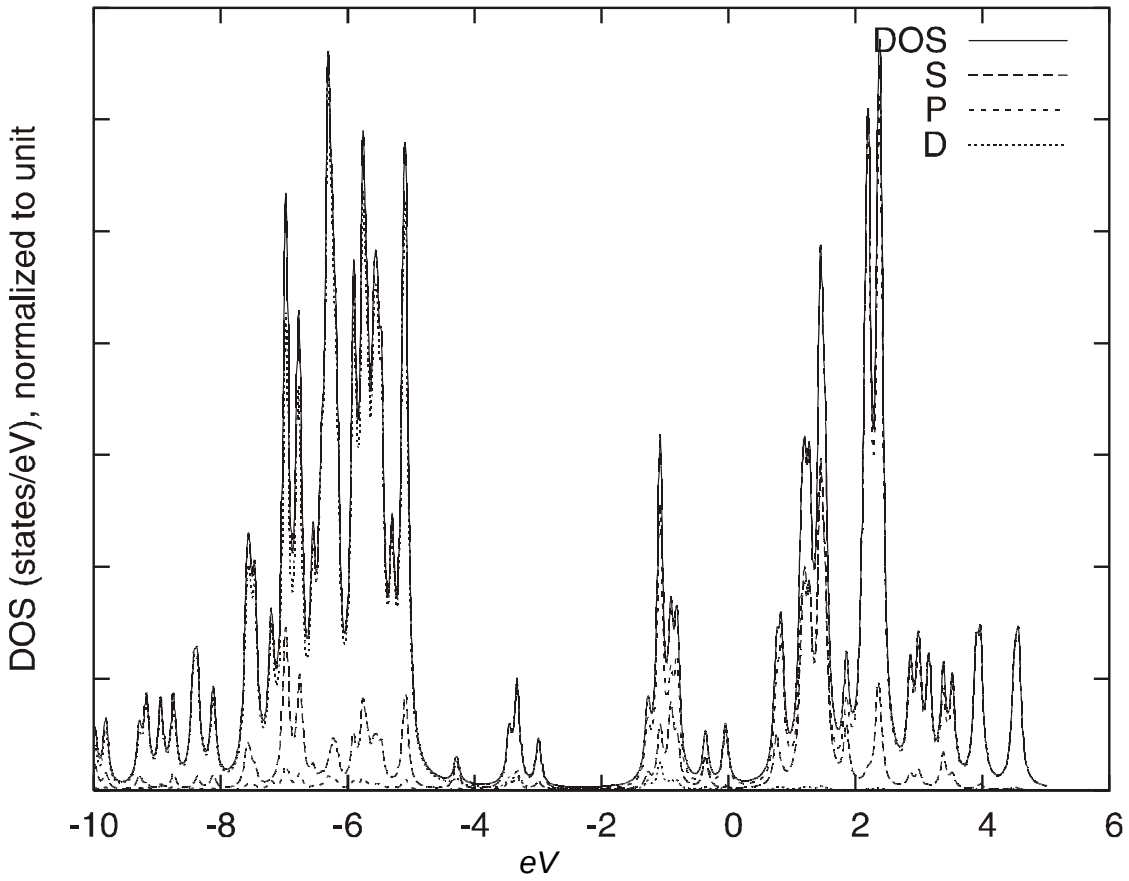

Figure 4aAS The alpha–spin density of states of triplet ECTB Pt_7 cluster. DOS is the total alpha–spin density of states. S, P and D are the partial alpha–spin density of states for angular momentum *s*, *p* and *d*.

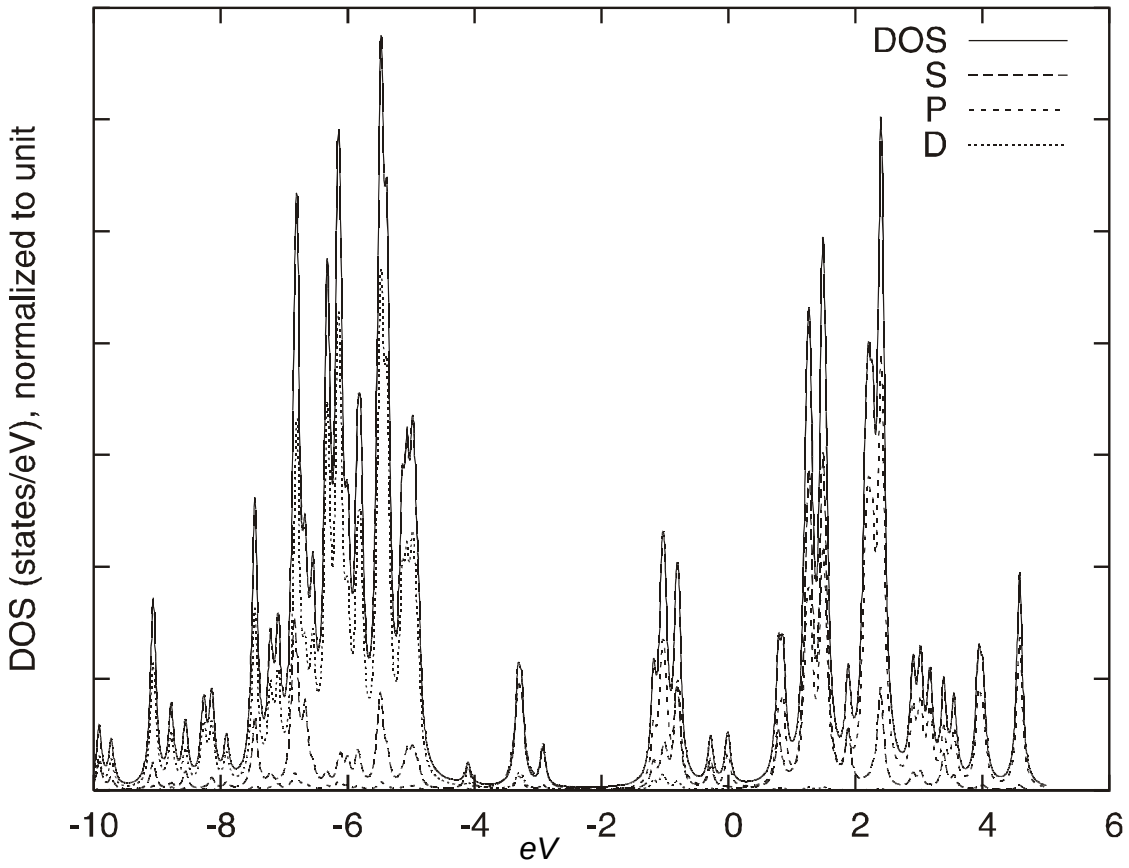

Figure 4aBS The beta−spin density of states of triplet ECTB Pt_7 cluster. DOS is the total beta−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

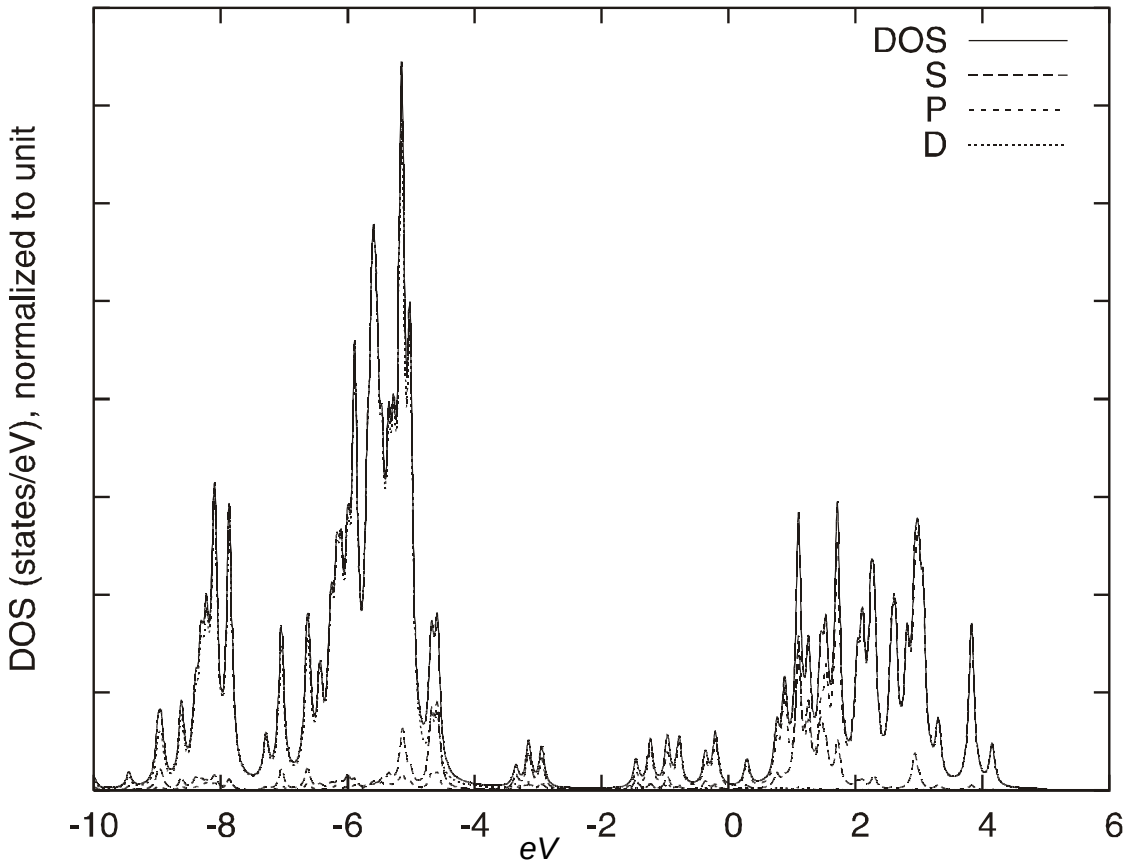

Figure 4bAS The alpha−spin density of states of quintet FCTB Pt_7 cluster. DOS is the total alpha−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

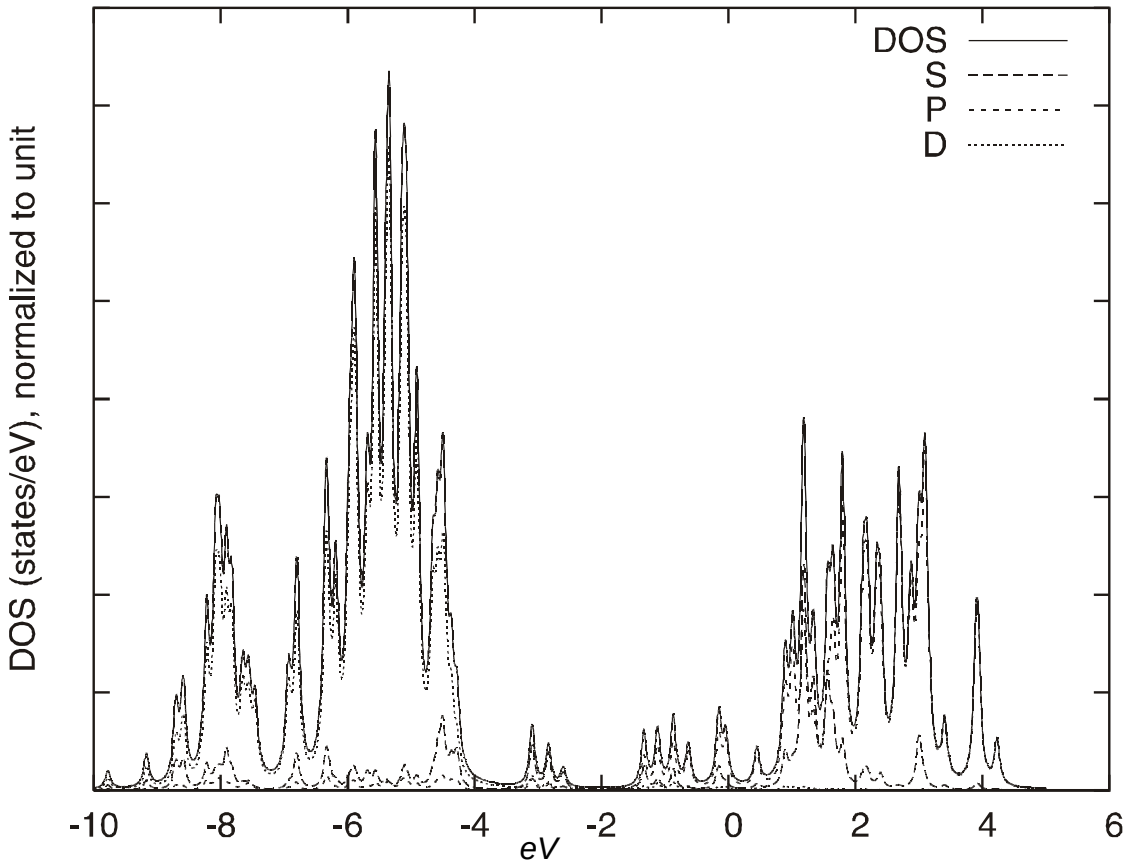

Figure 4bBS The beta−spin density of states of quintet FCTB Pt_7 cluster. DOS is the total beta−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

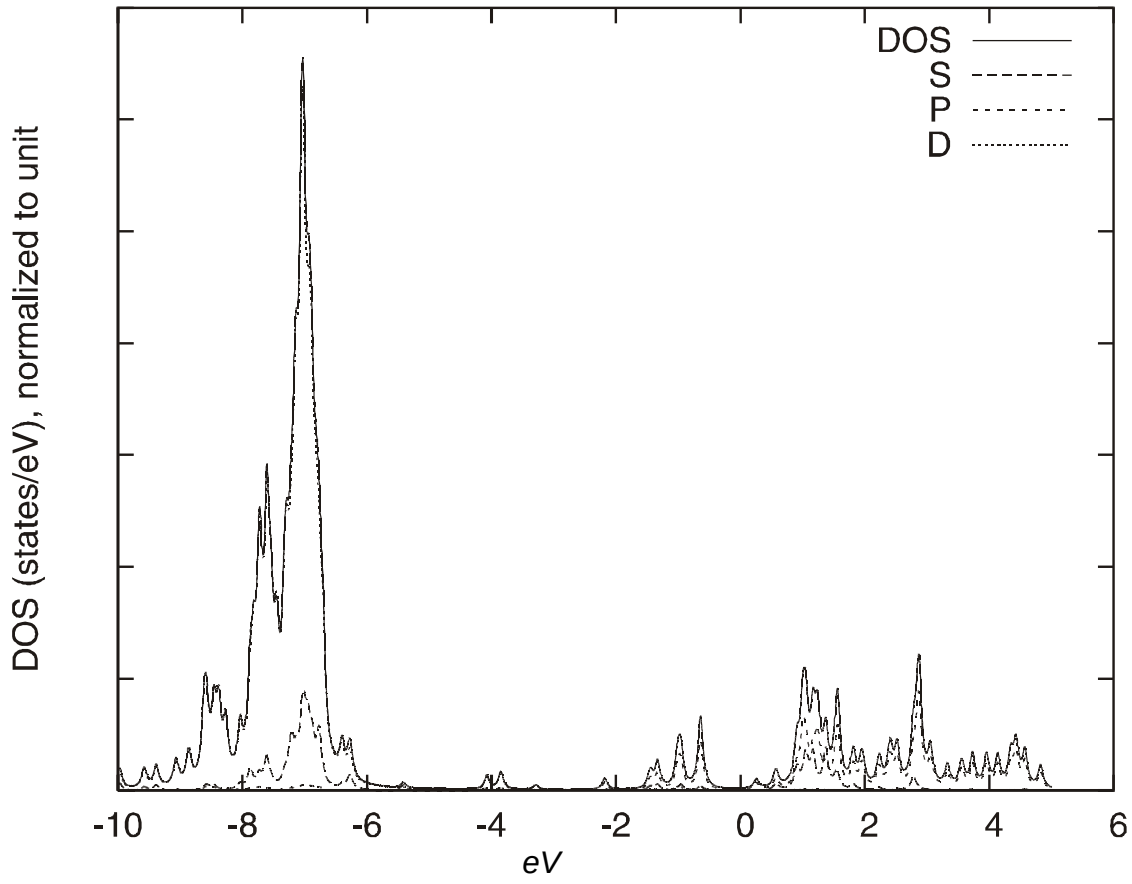

Figure 5aS The alpha−spin density of states of doublet ECR Au_7 cluster. DOS is the total alpha−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.

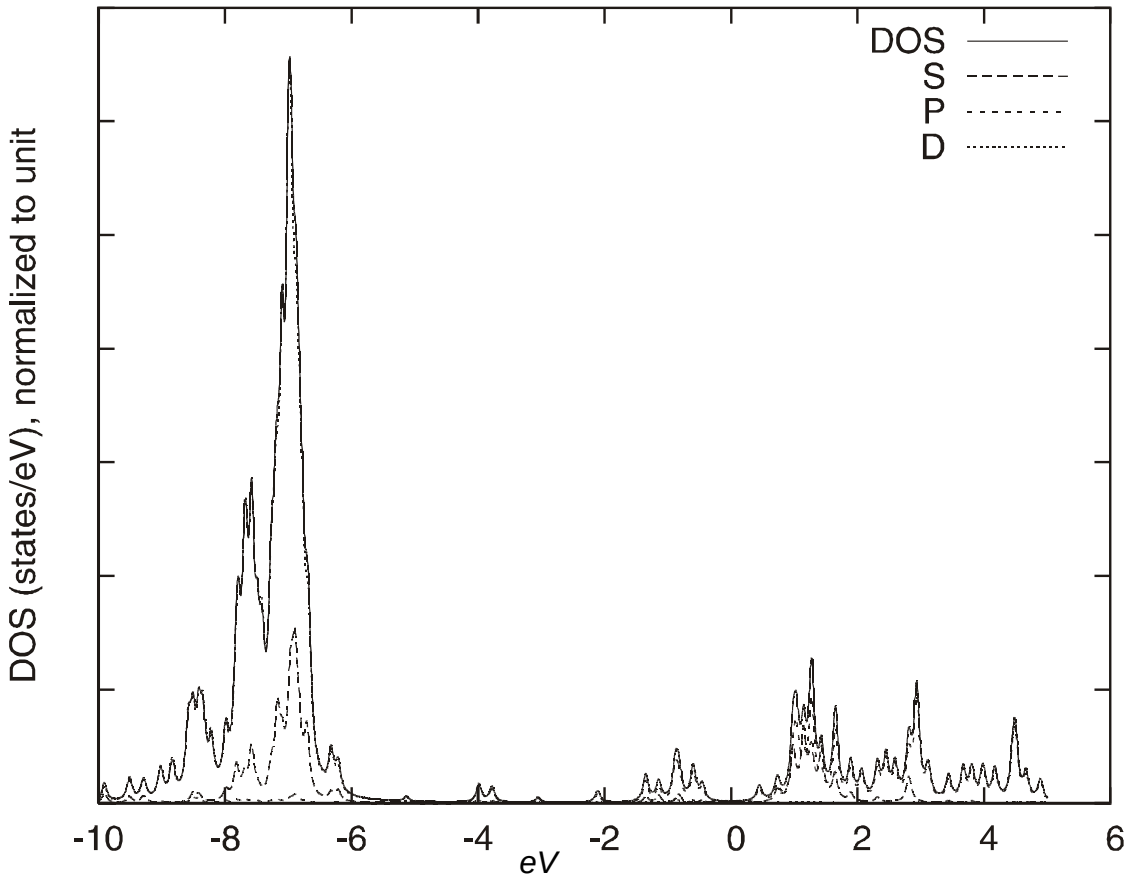

Figure 5bS The beta−spin density of states of doublet ECR Au_7 cluster. DOS is the total beta−spin density of states. S, P and D are the partial alpha−spin density of states for angular momentum *s*, *p* and *d*.