Supporting Information
for
Unusual Strain Effect of Pt-Based Face-Centered Tetragonal Core in Core/Shell Nanoparticles for Oxygen Reduction Reaction

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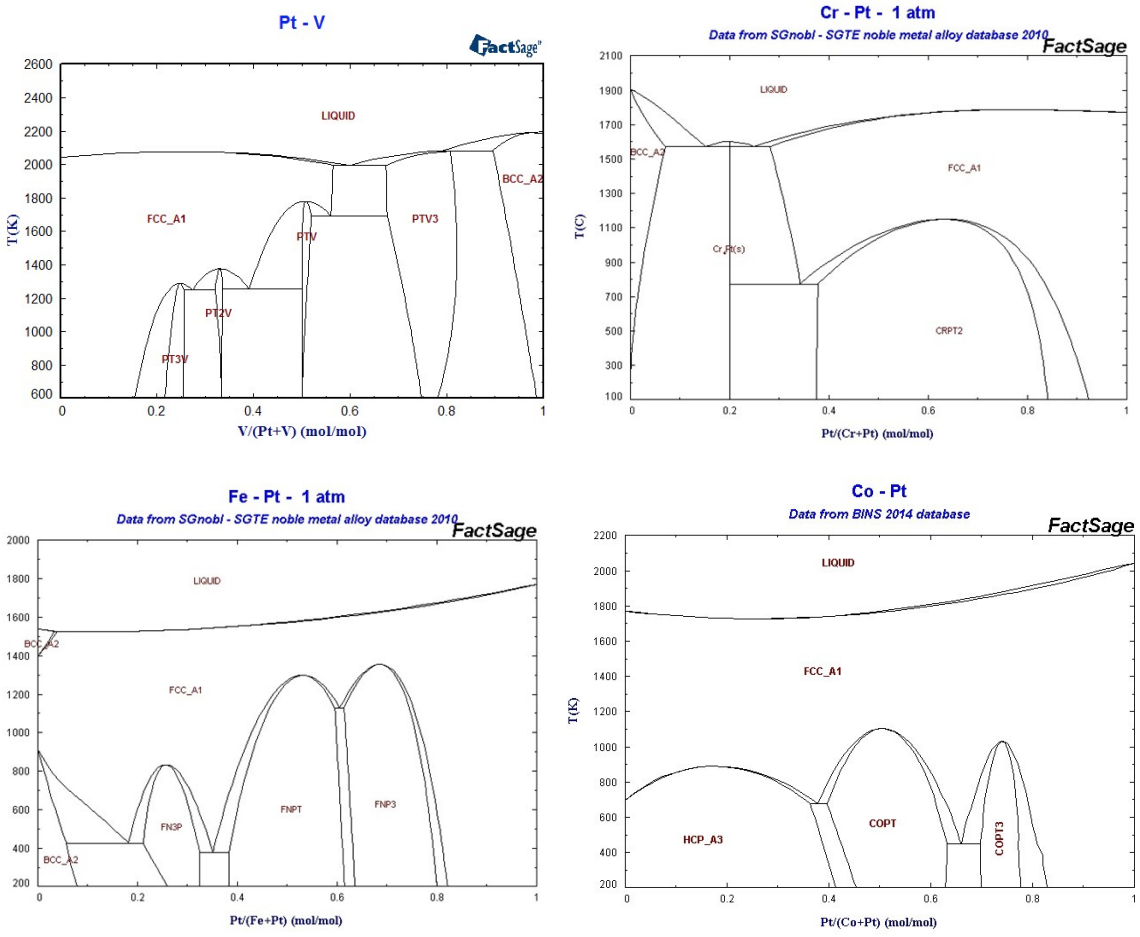
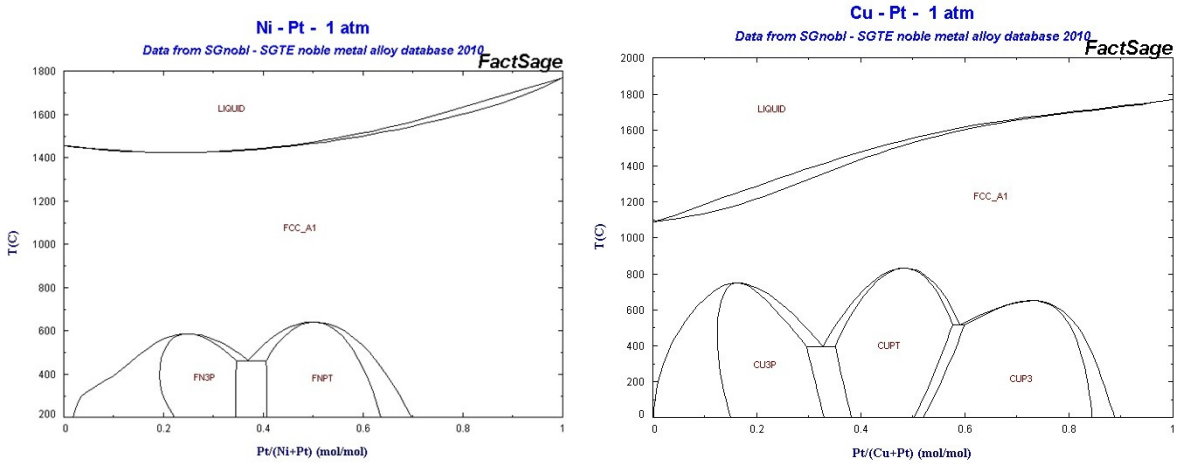
S1. Phase diagram of Pt-alloy:

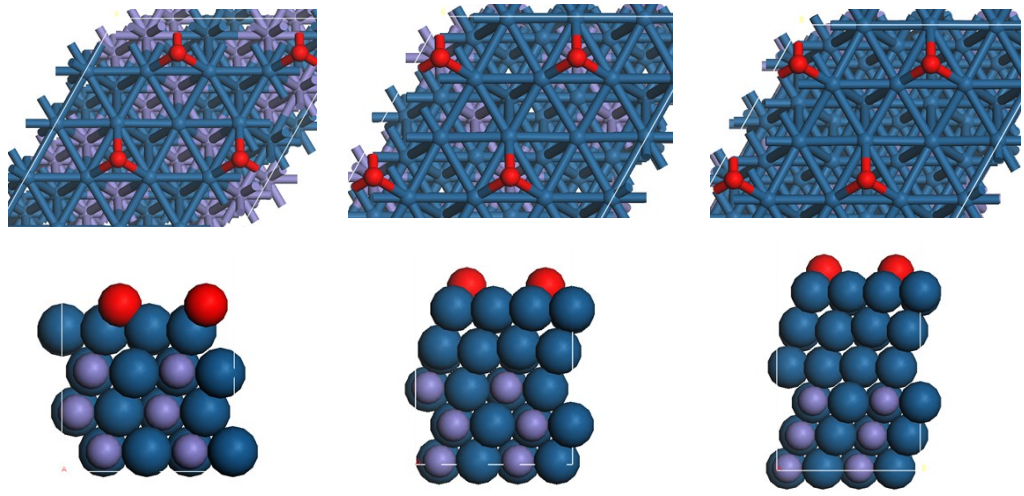
The phase diagram of Pt-M alloy for M=V, Cr, Fe, Co, Ni and Cu are from *FactSage*. The stability of the intermetallic Pt-M alloy can be estimated by their thermodynamic states with temperature and composition. Under equilibrium condition, the intermetallic phase of $Pt_{0.5}$-$M_{0.5}$ is stable below certain temperature, indicating by the double dome structure.



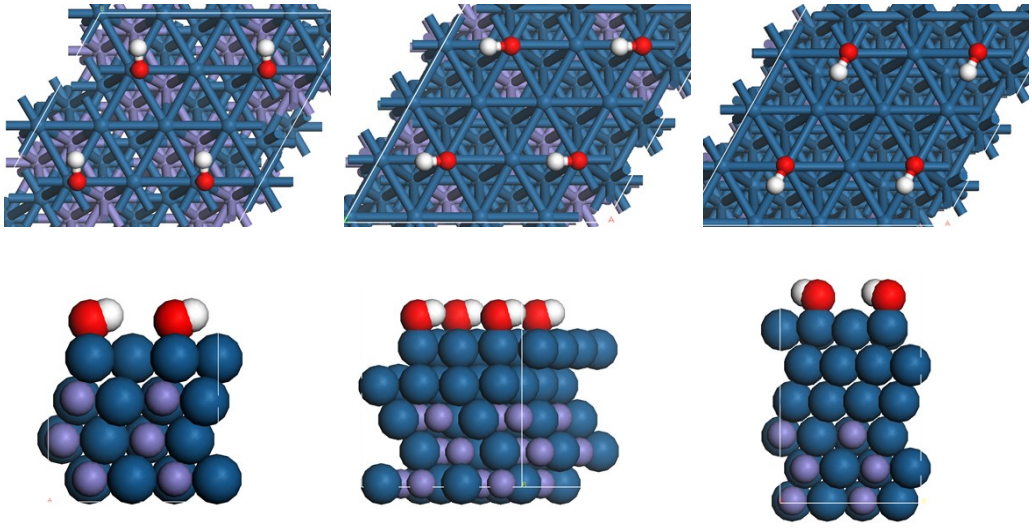


S2. Most stable structures of O*, OH* and OOH* on Pt/fct-PtM:

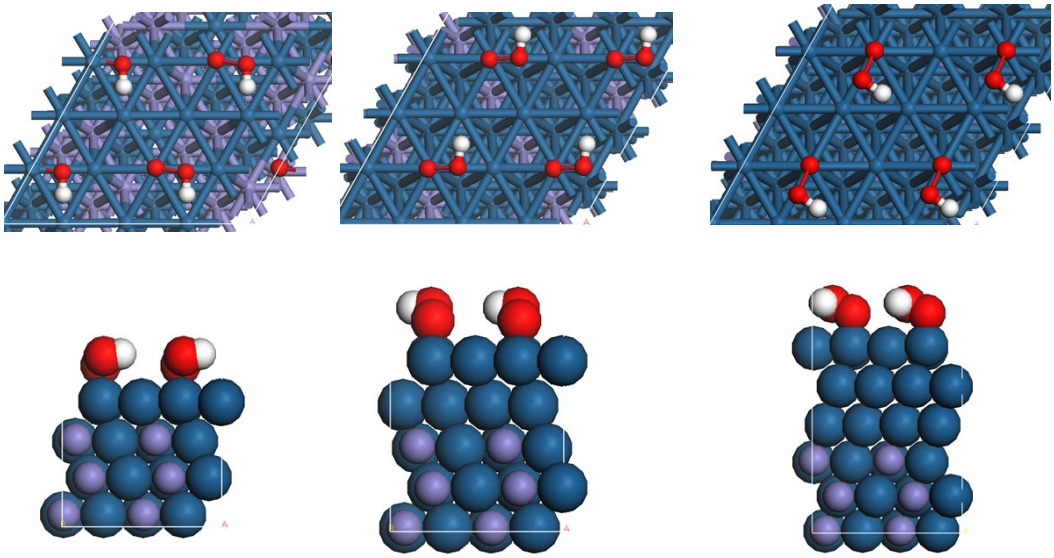
Using one, two and three layers of Pt on top of Pt-Fe as an example, the most stable structures for O*, OH* and OOH* adsorption: (we doubled the unit cell to (4x4) supercell for the illustration, shown with top and side views)



Most stable O* on 1, 2 and 3-Pt layers on fct-PtFe



Most stable OH* on 1, 2 and 3-Pt layers on fct-PtFe



Most stable OOH* on 1, 2 and 3-Pt layers on fct-PtFe

S3. Fractional coordinates for relaxed (111) facet of fct Pt-M (3 layers) with 1, 2 and 3 layers of Pt:

3+1: 3 layers of Pt-M and 1 layer Pt skin

3+2: 3 layers of Pt-M and 2 layers Pt skin

3+3: 3 layers of Pt-M and 3 layers Pt skin

a (Å) b (Å) c (Å) α(°) β (°) γ (°)

Pt-V:

3+1:

	5.472054	5.472054	25.000017	90.000000	90.000000	59.314232
V1	0.013678	0.513678	0.022619			
V2	0.685705	0.185705	0.106455			
V3	0.363577	0.863577	0.204267			
V4	0.513678	0.013678	0.022619			
V5	0.185715	0.685715	0.106461			
V6	0.863576	0.363576	0.204268			
Pt1	0.019594	0.519594	0.291099			
Pt2	0.519596	0.019596	0.291099			
Pt3	0.013678	0.013678	0.022619			
Pt4	0.686861	0.686870	0.111646			
Pt5	0.368831	0.368836	0.193293			
Pt6	0.023959	0.023947	0.289820			
Pt7	0.513678	0.513678	0.022619			
Pt8	0.186870	0.186861	0.111646			
Pt9	0.868836	0.868831	0.193293			
Pt10	0.523947	0.523959	0.289820			

3+2

	5.472054	5.472054	25.000017	90.000000	90.000000	59.314232
V1	0.351571	0.851571	0.022202			

V2 0.022399 0.522399 0.105608
V3 0.698556 0.198556 0.202191
V4 0.851571 0.351571 0.022202
V5 0.522441 0.022441 0.105616
V6 0.198556 0.698556 0.202193
Pt1 0.353627 0.853627 0.287919
Pt2 0.009091 0.509091 0.385952
Pt3 0.853629 0.353629 0.287921
Pt4 0.509088 0.009088 0.385954
Pt5 0.351571 0.351571 0.022202
Pt6 0.025369 0.025359 0.110991
Pt7 0.704515 0.704516 0.194021
Pt8 0.354616 0.354614 0.286785
Pt9 0.008726 0.008727 0.384014
Pt10 0.851571 0.851571 0.022202
Pt11 0.525359 0.525369 0.110991
Pt12 0.204516 0.204515 0.194021
Pt13 0.854614 0.854616 0.286785
Pt14 0.508727 0.508726 0.384014

3+3
5.472054 5.472054 27.000046 90.000000 90.000000 59.314232
V1 0.689464 0.189464 0.021949
V2 0.361741 0.861742 0.099796
V3 0.035083 0.535116 0.188511
V4 0.189464 0.689464 0.021949
V5 0.861718 0.361730 0.099792
V6 0.535098 0.035083 0.188508
Pt1 0.691727 0.191768 0.269028
Pt2 0.352621 0.852600 0.358681
Pt3 0.016842 0.516834 0.447667
Pt4 0.191760 0.691726 0.269029
Pt5 0.852600 0.352610 0.358681
Pt6 0.516841 0.016835 0.447667
Pt7 0.689464 0.689464 0.021949
Pt8 0.363304 0.363319 0.104020
Pt9 0.041556 0.041577 0.180948
Pt10 0.694738 0.694742 0.268196
Pt11 0.352994 0.352992 0.358212
Pt12 0.015987 0.015981 0.448235
Pt13 0.189464 0.189464 0.021949
Pt14 0.863293 0.863310 0.104013
Pt15 0.541596 0.541597 0.180949
Pt16 0.194733 0.194736 0.268191
Pt17 0.852995 0.852988 0.358215
Pt18 0.515989 0.515979 0.448236

Pt-Cr
3+1
5.395720 5.395720 24.999983 90.000000 90.000000 59.441555

Cr1 0.011160 0.511160 0.022595
Cr2 0.694569 0.194568 0.110169
Cr3 0.376863 0.876881 0.203622
Cr4 0.511160 0.011160 0.022595
Cr5 0.194578 0.694555 0.110171
Cr6 0.876876 0.376878 0.203622
Pt1 0.048663 0.548739 0.295227
Pt2 0.548683 0.048709 0.295227
Pt3 0.011160 0.011160 0.022595
Pt4 0.692440 0.692440 0.114183
Pt5 0.380034 0.380098 0.197463
Pt6 0.050930 0.050964 0.292782
Pt7 0.511160 0.511160 0.022595
Pt8 0.192409 0.192417 0.114186
Pt9 0.880089 0.880030 0.197474
Pt10 0.550893 0.550952 0.292741

3+2:
5.395720 5.395720 25.000011 90.000000 90.000000 59.441555
Cr1 0.348213 0.848213 0.022163
Cr2 0.026877 0.526877 0.108584
Cr3 0.705164 0.205164 0.203653
Cr4 0.848213 0.348213 0.022163
Cr5 0.526883 0.026883 0.108587
Cr6 0.205175 0.705175 0.203655
Pt1 0.368582 0.868582 0.291437
Pt2 0.024827 0.524827 0.389475
Pt3 0.868583 0.368583 0.291435
Pt4 0.524825 0.024825 0.389479
Pt5 0.348213 0.348213 0.022163
Pt6 0.025952 0.025910 0.113943
Pt7 0.711140 0.711154 0.196534
Pt8 0.369525 0.369531 0.289544
Pt9 0.024235 0.024236 0.388210
Pt10 0.848213 0.848213 0.022163
Pt11 0.525910 0.525952 0.113943
Pt12 0.211154 0.211140 0.196534
Pt13 0.869531 0.869525 0.289544
Pt14 0.524236 0.524235 0.388210

3+3:
5.395720 5.395720 27.000038 90.000000 90.000000 59.441555
Cr1 0.685267 0.185267 0.021915
Cr2 0.367620 0.867053 0.102573
Cr3 0.047280 0.546264 0.189469
Cr4 0.185267 0.685267 0.021915
Cr5 0.867644 0.367083 0.102582
Cr6 0.547243 0.046256 0.189452
Pt1 0.715210 0.213468 0.272857

Pt2 0.370991 0.867172 0.362724
Pt3 0.022606 0.519664 0.452560
Pt4 0.215224 0.713446 0.272848
Pt5 0.870944 0.367136 0.362656
Pt6 0.522619 0.019659 0.452729
Pt7 0.685267 0.685267 0.021915
Pt8 0.366242 0.365589 0.106614
Pt9 0.051453 0.050630 0.183945
Pt10 0.716995 0.715207 0.270351
Pt11 0.371236 0.367414 0.362199
Pt12 0.022183 0.019267 0.453718
Pt13 0.185267 0.185267 0.021915
Pt14 0.866280 0.865603 0.106621
Pt15 0.551489 0.550608 0.183948
Pt16 0.216993 0.215190 0.270354
Pt17 0.871238 0.867366 0.362163
Pt18 0.522172 0.519279 0.453828

Pt-Fe:
3+1:
5.400027 5.400027 24.999956 90.000000 90.000000 60.770180
Fe1 0.984296 0.484296 0.000000
Fe2 0.661045 0.161045 0.085246
Fe3 0.339928 0.839928 0.178829
Fe4 0.484296 0.984296 0.000000
Fe5 0.161051 0.661051 0.085245
Fe6 0.839927 0.339927 0.178828
Pt1 0.002362 0.502362 0.268696
Pt2 0.502363 0.002363 0.268696
Pt3 0.984296 0.984296 0.000000
Pt4 0.661242 0.661241 0.087794
Pt5 0.341583 0.341584 0.172123
Pt6 0.004803 0.004803 0.266750
Pt7 0.484296 0.484296 0.000000
Pt8 0.161241 0.161242 0.087794
Pt9 0.841584 0.841583 0.172123
Pt10 0.504803 0.504803 0.266750

3+2:
5.400027 5.400027 25.000042 90.000000 90.000000 60.770180
Fe1 0.312395 0.812395 0.008160
Fe2 0.989657 0.489657 0.093537
Fe3 0.667616 0.167616 0.185843
Fe4 0.812395 0.312395 0.008160
Fe5 0.489675 0.989675 0.093536
Fe6 0.167620 0.667620 0.185841
Pt1 0.330892 0.830892 0.274828
Pt2 0.989725 0.489725 0.373336
Pt3 0.830894 0.330894 0.274829
Pt4 0.489724 0.989724 0.373332

Pt5 0.312395 0.312395 0.008160
Pt6 0.990507 0.990510 0.096117
Pt7 0.670563 0.670563 0.181161
Pt8 0.330983 0.331003 0.273128
Pt9 0.988764 0.988760 0.370195
Pt10 0.812395 0.812395 0.008160
Pt11 0.490510 0.490507 0.096117
Pt12 0.170563 0.170563 0.181161
Pt13 0.831003 0.830983 0.273128
Pt14 0.488760 0.488764 0.370195

3+3:
5.400027 5.400027 27.000027 90.000000 90.000000 60.770180
Fe1 0.640494 0.140494 0.005476
Fe2 0.319334 0.819334 0.085070
Fe3 0.994118 0.494118 0.169595
Fe4 0.140494 0.640494 0.005476
Fe5 0.819333 0.319333 0.085071
Fe6 0.494117 0.994117 0.169595
Pt1 0.659398 0.159398 0.253446
Pt2 0.325894 0.825894 0.342512
Pt3 0.993621 0.493621 0.431398
Pt4 0.159402 0.659402 0.253447
Pt5 0.825893 0.325893 0.342513
Pt6 0.493621 0.993621 0.431398
Pt7 0.640494 0.640494 0.005476
Pt8 0.319719 0.319728 0.086453
Pt9 0.996513 0.996514 0.165968
Pt10 0.661189 0.661190 0.251006
Pt11 0.326086 0.326086 0.341746
Pt12 0.993123 0.993124 0.432599
Pt13 0.140494 0.140494 0.005476
Pt14 0.819728 0.819718 0.086453
Pt15 0.496514 0.496513 0.165968
Pt16 0.161190 0.161189 0.251006
Pt17 0.826086 0.826086 0.341746
Pt18 0.493124 0.493123 0.432599

Pt-Co:
3+1:
5.334154 5.334154 24.999969 90.000000 90.000000 60.797485
Co1 0.983733 0.483733 0.008402
Co2 0.657099 0.157099 0.093679
Co3 0.331213 0.831213 0.183658
Co4 0.483733 0.983733 0.008402
Co5 0.157100 0.657100 0.093679
Co6 0.831213 0.331213 0.183658
Pt1 0.995377 0.495377 0.274721
Pt2 0.495377 0.995377 0.274721
Pt3 0.983733 0.983733 0.008402

Pt4 0.657558 0.657558 0.095261
Pt5 0.334692 0.334690 0.178967
Pt6 0.997305 0.997305 0.272670
Pt7 0.483733 0.483733 0.008402
Pt8 0.157558 0.157558 0.095261
Pt9 0.834690 0.834692 0.178967
Pt10 0.497305 0.497305 0.272670

3+2:
5.334154 5.334154 25.000027 90.000000 90.000000 60.797485
Co1 0.311644 0.811644 0.006871
Co2 0.983218 0.483218 0.091138
Co3 0.659240 0.159240 0.182463
Co4 0.811644 0.311644 0.006871
Co5 0.483214 0.983214 0.091137
Co6 0.159242 0.659242 0.182464
Pt1 0.323301 0.823301 0.271816
Pt2 0.980643 0.480643 0.370831
Pt3 0.823302 0.323302 0.271818
Pt4 0.480640 0.980640 0.370828
Pt5 0.311644 0.311644 0.006871
Pt6 0.984105 0.984089 0.094045
Pt7 0.664620 0.664636 0.177478
Pt8 0.324020 0.324036 0.270225
Pt9 0.980105 0.980106 0.368464
Pt10 0.811644 0.811644 0.006871
Pt11 0.484089 0.484105 0.094045
Pt12 0.164636 0.164620 0.177478
Pt13 0.824036 0.824020 0.270225
Pt14 0.480106 0.480105 0.368464

3+3:
5.334154 5.334154 26.999983 90.000000 90.000000 60.797485
Co1 0.639555 0.139555 0.007725
Co2 0.310680 0.810680 0.085750
Co3 0.989211 0.489211 0.170837
Co4 0.139555 0.639555 0.007725
Co5 0.810689 0.310688 0.085752
Co6 0.489213 0.989212 0.170838
Pt1 0.654518 0.154517 0.254129
Pt2 0.317144 0.817149 0.343852
Pt3 0.978075 0.478075 0.433579
Pt4 0.154518 0.654517 0.254127
Pt5 0.817147 0.317151 0.343852
Pt6 0.478078 0.978077 0.433578
Pt7 0.639555 0.639555 0.007725
Pt8 0.312013 0.312030 0.088556
Pt9 0.992787 0.992756 0.165790
Pt10 0.655560 0.655556 0.251819
Pt11 0.317640 0.317648 0.343834

Pt12 0.978017 0.978020 0.436065
Pt13 0.139555 0.139555 0.007725
Pt14 0.812031 0.812012 0.088556
Pt15 0.492757 0.492787 0.165790
Pt16 0.155556 0.155560 0.251819
Pt17 0.817646 0.817640 0.343834
Pt18 0.478020 0.478017 0.436064

Pt-Ni:
3+1:
5.295301 5.295301 24.999975 90.000000 90.000000 61.940582
Ni1 0.959721 0.459721 0.005588
Ni2 0.642997 0.142997 0.091617
Ni3 0.322410 0.822410 0.178672
Ni4 0.459721 0.959721 0.005588
Ni5 0.142997 0.642997 0.091617
Ni6 0.822411 0.322411 0.178671
Pt1 0.997310 0.497310 0.272126
Pt2 0.497310 0.997310 0.272128
Pt3 0.959721 0.959721 0.005588
Pt4 0.642819 0.642819 0.092131
Pt5 0.324579 0.324579 0.176606
Pt6 0.998843 0.998843 0.268330
Pt7 0.459721 0.459721 0.005588
Pt8 0.142819 0.142819 0.092131
Pt9 0.824579 0.824579 0.176606
Pt10 0.498843 0.498843 0.268330

3+2:
5.295301 5.295301 25.000002 90.000000 90.000000 61.940582
Ni1 0.279628 0.779628 0.005361
Ni2 0.964556 0.464555 0.091196
Ni3 0.645009 0.145009 0.179191
Ni4 0.779628 0.279628 0.005361
Ni5 0.464562 0.964562 0.091198
Ni6 0.145005 0.645005 0.179191
Pt1 0.313448 0.813448 0.270411
Pt2 0.975329 0.475329 0.369784
Pt3 0.813451 0.313451 0.270410
Pt4 0.475307 0.975307 0.369785
Pt5 0.279628 0.279628 0.005361
Pt6 0.964076 0.964067 0.092318
Pt7 0.648051 0.648043 0.176496
Pt8 0.314155 0.314165 0.268454
Pt9 0.974619 0.974589 0.366515
Pt10 0.779628 0.779628 0.005361
Pt11 0.464067 0.464076 0.092318
Pt12 0.148043 0.148051 0.176496
Pt13 0.814165 0.814155 0.268454
Pt14 0.474589 0.474619 0.366515

3+3:
5.295301 5.295301 27.000027 90.000000 90.000000 61.940582
Ni1 0.599535 0.099535 0.005477
Ni2 0.283898 0.783898 0.084766
Ni3 0.965768 0.465768 0.166414
Ni4 0.099535 0.599535 0.005477
Ni5 0.783898 0.283898 0.084764
Ni6 0.465760 0.965760 0.166414
Pt1 0.638981 0.138981 0.251882
Pt2 0.309679 0.809679 0.343083
Pt3 0.997529 0.497529 0.430218
Pt4 0.138982 0.638982 0.251883
Pt5 0.809679 0.309679 0.343083
Pt6 0.497529 0.997529 0.430219
Pt7 0.599535 0.599535 0.005477
Pt8 0.283800 0.283803 0.085907
Pt9 0.968170 0.968170 0.164119
Pt10 0.639903 0.639901 0.249067
Pt11 0.310371 0.310371 0.340356
Pt12 0.997270 0.997270 0.436419
Pt13 0.099535 0.099535 0.005477
Pt14 0.783803 0.783800 0.085907
Pt15 0.468170 0.468170 0.164119
Pt16 0.139901 0.139903 0.249067
Pt17 0.810371 0.810371 0.340356
Pt18 0.497270 0.497270 0.436419

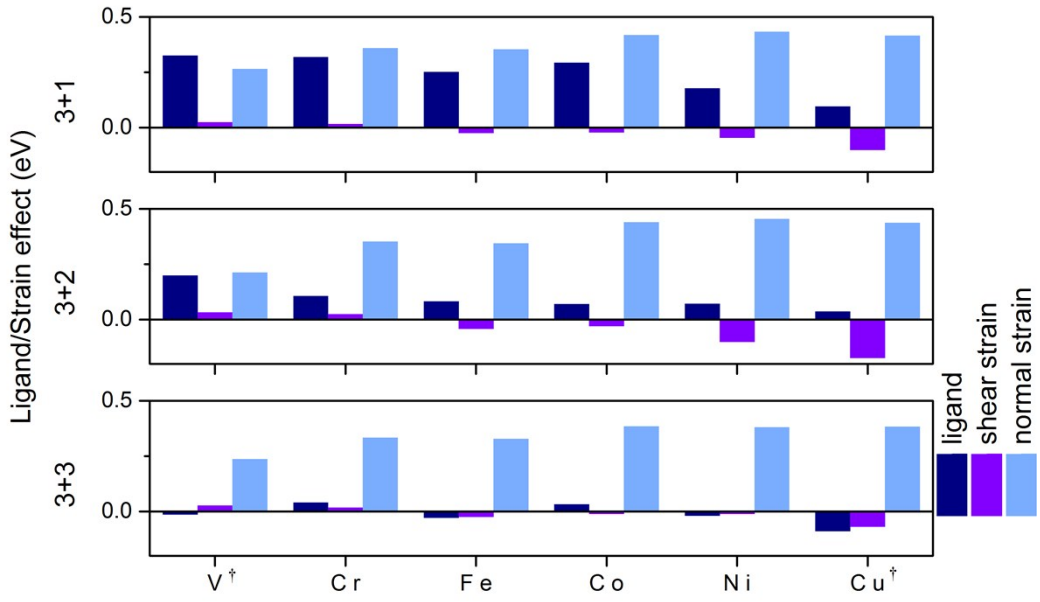
Pt-Cu:
3+1:
5.336905 5.336905 25.000038 90.000000 90.000000 62.847446
Cu1 0.940071 0.440071 0.022271
Cu2 0.615228 0.115227 0.108871
Cu3 0.294233 0.794233 0.198688
Cu4 0.440071 0.940071 0.022271
Cu5 0.115227 0.615227 0.108872
Cu6 0.794233 0.294233 0.198688
Pt1 0.960045 0.460045 0.289561
Pt2 0.460046 0.960045 0.289561
Pt3 0.940071 0.940071 0.022271
Pt4 0.614992 0.614991 0.110689
Pt5 0.295597 0.295596 0.195658
Pt6 0.960911 0.960911 0.288204
Pt7 0.440071 0.440071 0.022271
Pt8 0.114991 0.114992 0.110689
Pt9 0.795596 0.795597 0.195658
Pt10 0.460912 0.460910 0.288204

3+2:
5.336905 5.336905 24.999985 90.000000 90.000000 62.847446

Cu1 0.253429 0.753428 0.022091
Cu2 0.928553 0.428552 0.109371
Cu3 0.607020 0.107019 0.198688
Cu4 0.753429 0.253428 0.022091
Cu5 0.428554 0.928553 0.109370
Cu6 0.107020 0.607020 0.198688
Pt1 0.279988 0.779988 0.289302
Pt2 0.949160 0.449160 0.388947
Pt3 0.779988 0.279988 0.289302
Pt4 0.449160 0.949160 0.388947
Pt5 0.253429 0.253428 0.022091
Pt6 0.928044 0.928044 0.110778
Pt7 0.609321 0.609320 0.196409
Pt8 0.279781 0.279781 0.288535
Pt9 0.948329 0.948330 0.384379
Pt10 0.753429 0.753428 0.022091
Pt11 0.428044 0.428043 0.110778
Pt12 0.109321 0.109321 0.196409
Pt13 0.779781 0.779781 0.288535
Pt14 0.448330 0.448329 0.384379

3+3:
5.336905 5.336905 27.000032 90.000000 90.000000 62.847446
Cu1 0.566786 0.066785 0.022033
Cu2 0.241103 0.741102 0.102278
Cu3 0.919951 0.419951 0.185616
Cu4 0.066786 0.566785 0.022033
Cu5 0.741103 0.241103 0.102278
Cu6 0.419953 0.919950 0.185616
Pt1 0.594954 0.094953 0.268058
Pt2 0.295949 0.795950 0.361118
Pt3 0.001537 0.501538 0.446306
Pt4 0.094953 0.594953 0.268058
Pt5 0.795949 0.295949 0.361118
Pt6 0.501537 0.001538 0.446306
Pt7 0.566786 0.566785 0.022033
Pt8 0.240795 0.240795 0.104004
Pt9 0.922694 0.922692 0.182898
Pt10 0.595156 0.595155 0.269773
Pt11 0.296674 0.296675 0.356635
Pt12 0.000974 0.000974 0.452359
Pt13 0.066786 0.066785 0.022033
Pt14 0.740797 0.740794 0.104004
Pt15 0.422693 0.422691 0.182898
Pt16 0.095156 0.095155 0.269773
Pt17 0.796674 0.796675 0.356635
Pt18 0.500974 0.500974 0.452359

S4. Ligand, shear and normal strain decomposition:


Ligand/Strain effect (eV)
0.5
0.0
3+1
3+2
3+3
V†
Cr
Fe
Co
Ni
Cu†
ligand
shear strain
normal strain