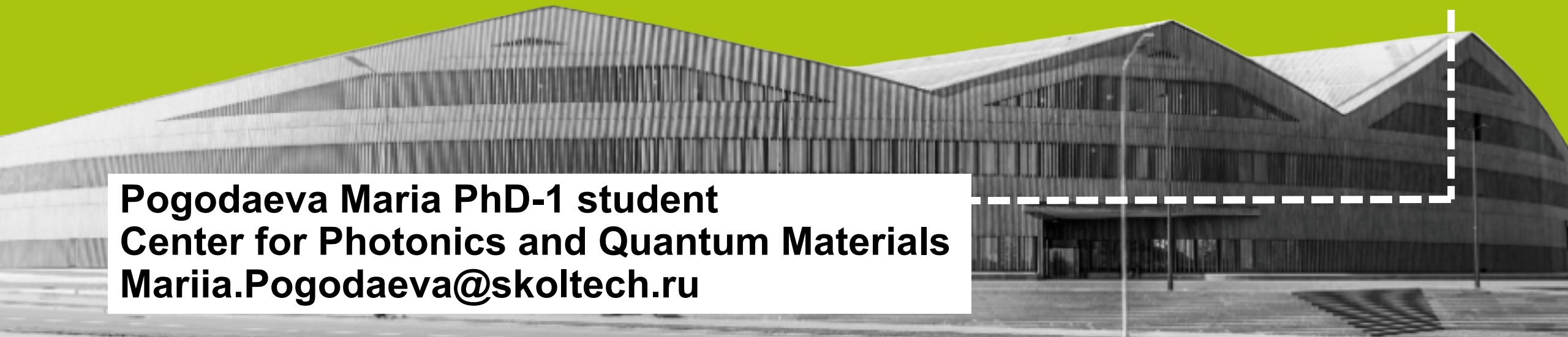
Final project

^{27}Co clusters. Magnetism. Optical properties.



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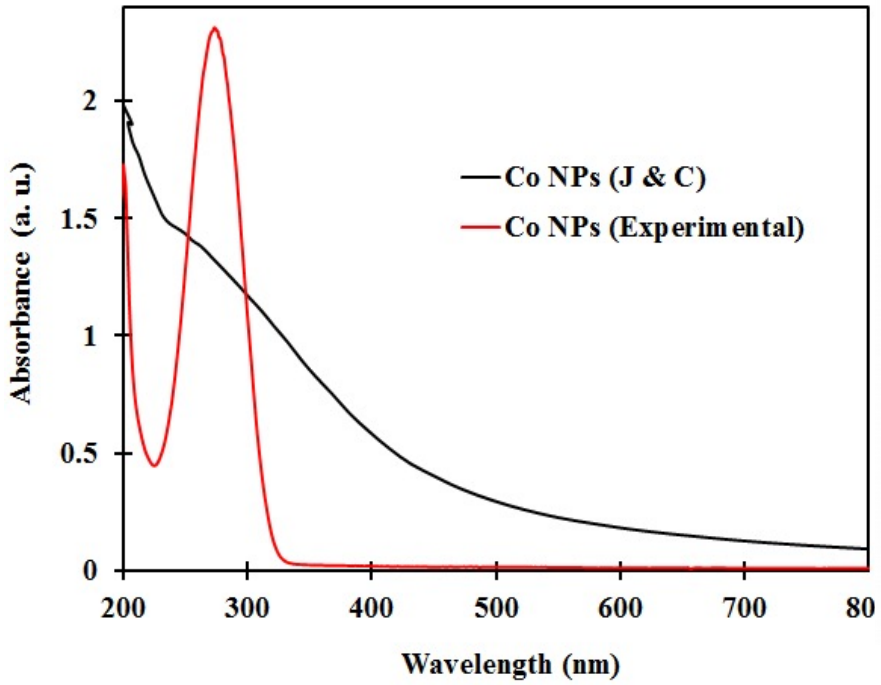
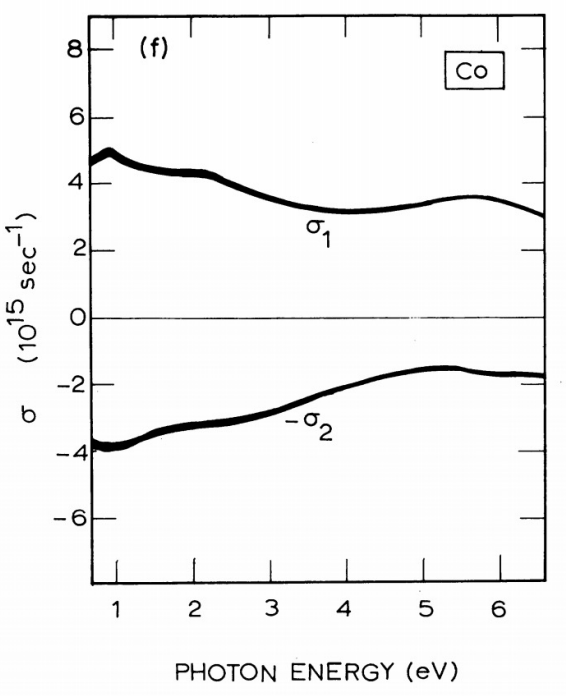
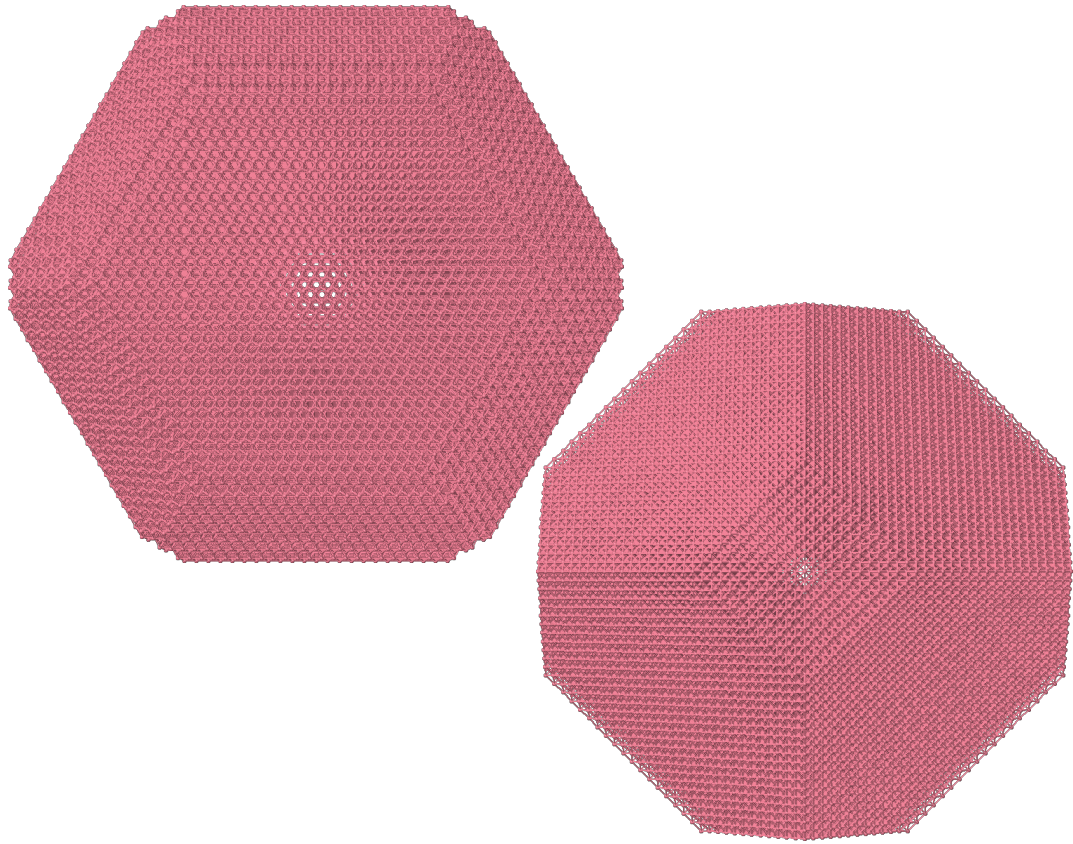
Problem statement

is coming from recent experimental observation of unexpected optical and magnetic properties for Co nanoparticles.
Specifically,

$$\sigma_{ext} = 9\frac{\omega\varepsilon_m^{1/2}}{c}V\frac{\varepsilon_m\varepsilon_2(\omega)}{\left[\varepsilon_1(\omega)+2\varepsilon_m\right]^2+\varepsilon_2^2(\omega)}$$



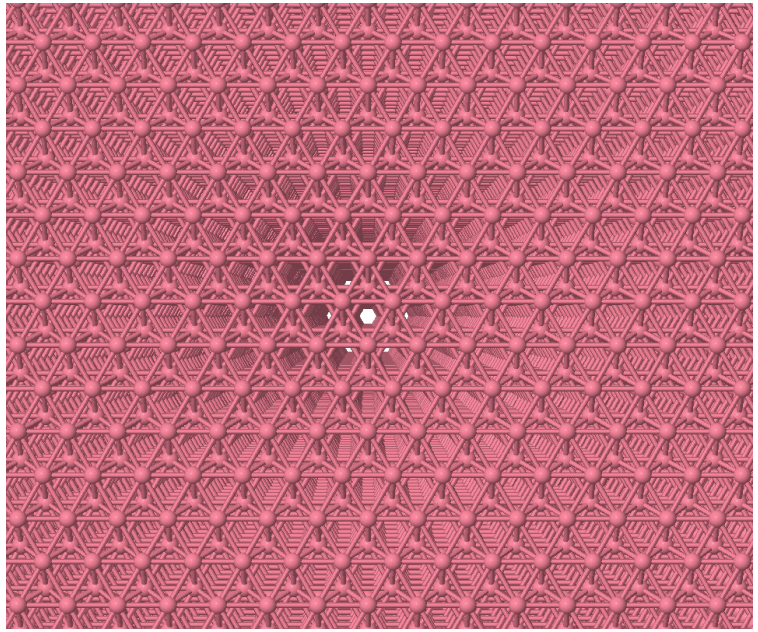




H.L. Bhata, A.E. Aliev, & V.P. Drachev, New mechanism of plasmons specific for spin-polarized nanoparticles.
SCIENTIFIC REPORTS *9, 2019 (2019)*

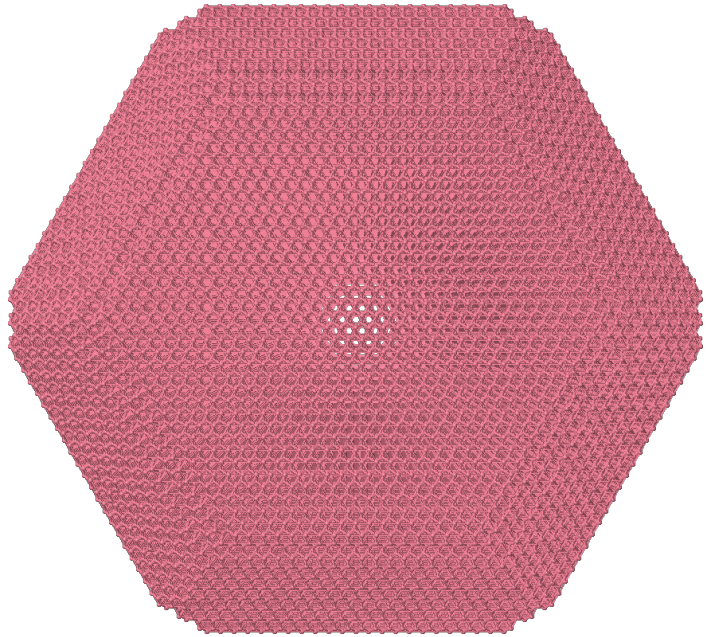
Johnson, P. B., and Christy, R. W. *Phys. Rev.* **9**, 5056 (1974).

Methods



Bulk. ABINIT

- Relaxation
- Magnetic moment
- Dielectric function

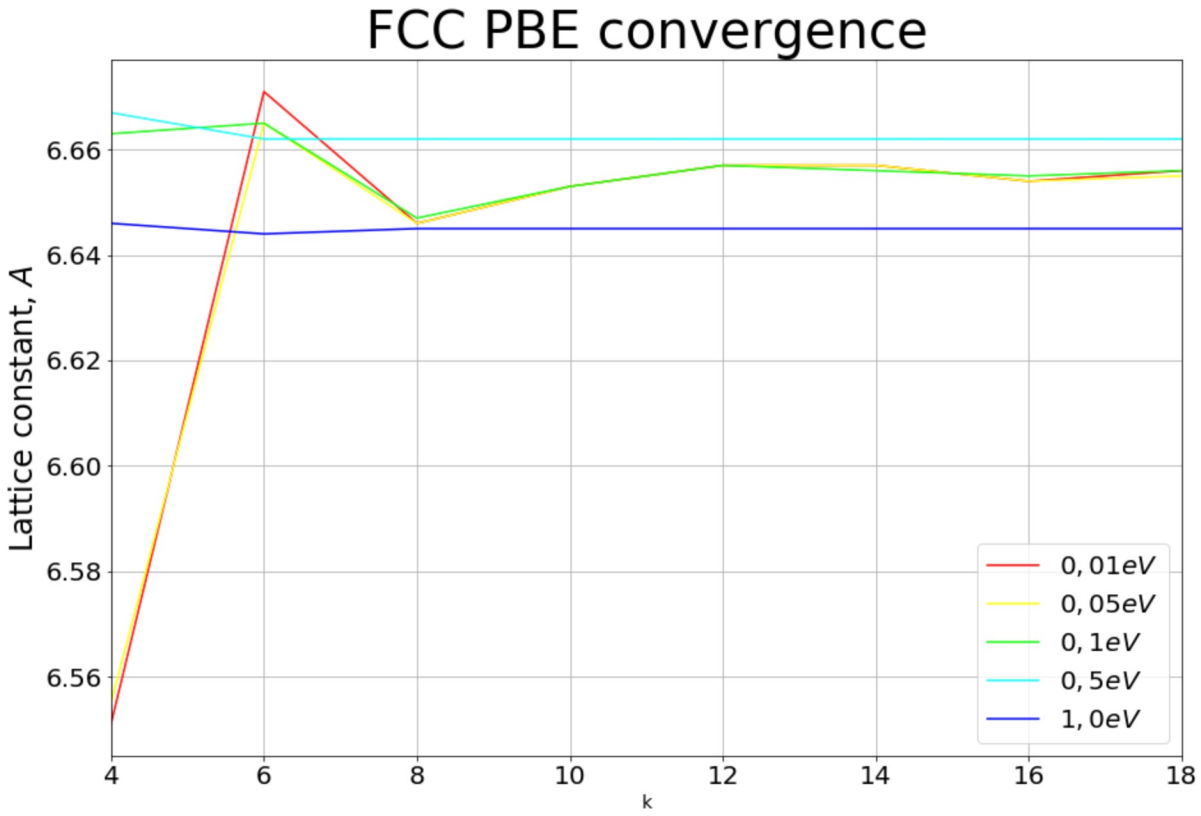


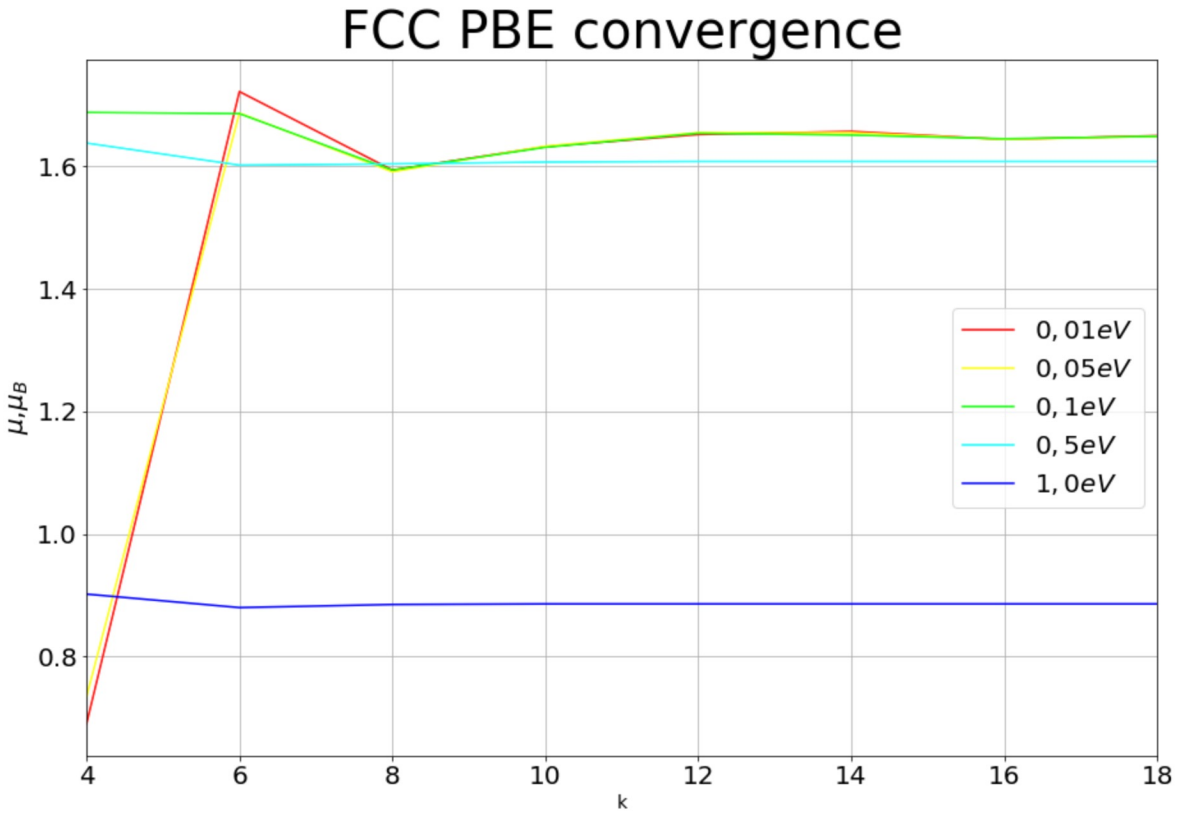
Cluster. FHI-aims

- Wulff construction
- Relaxation
- Magnetic moment

ABINIT

ABINIT results.
Parameters convergence w/ respect to k-point mesh
FCC

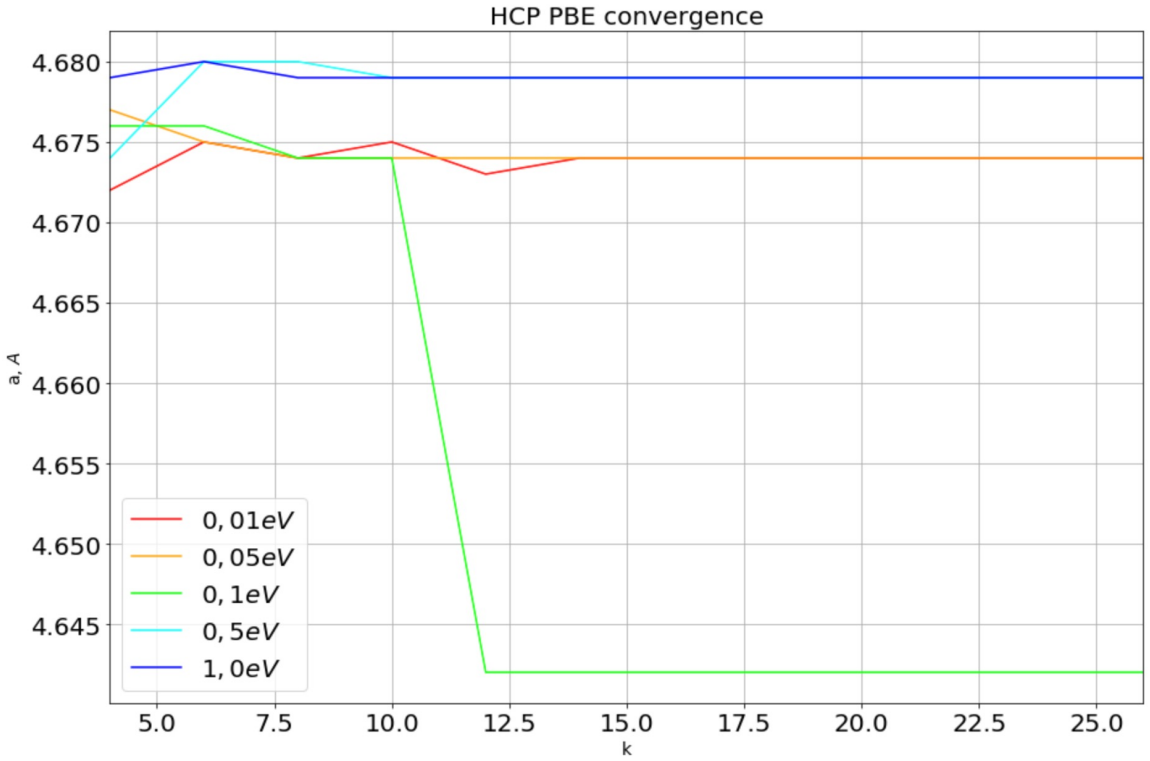


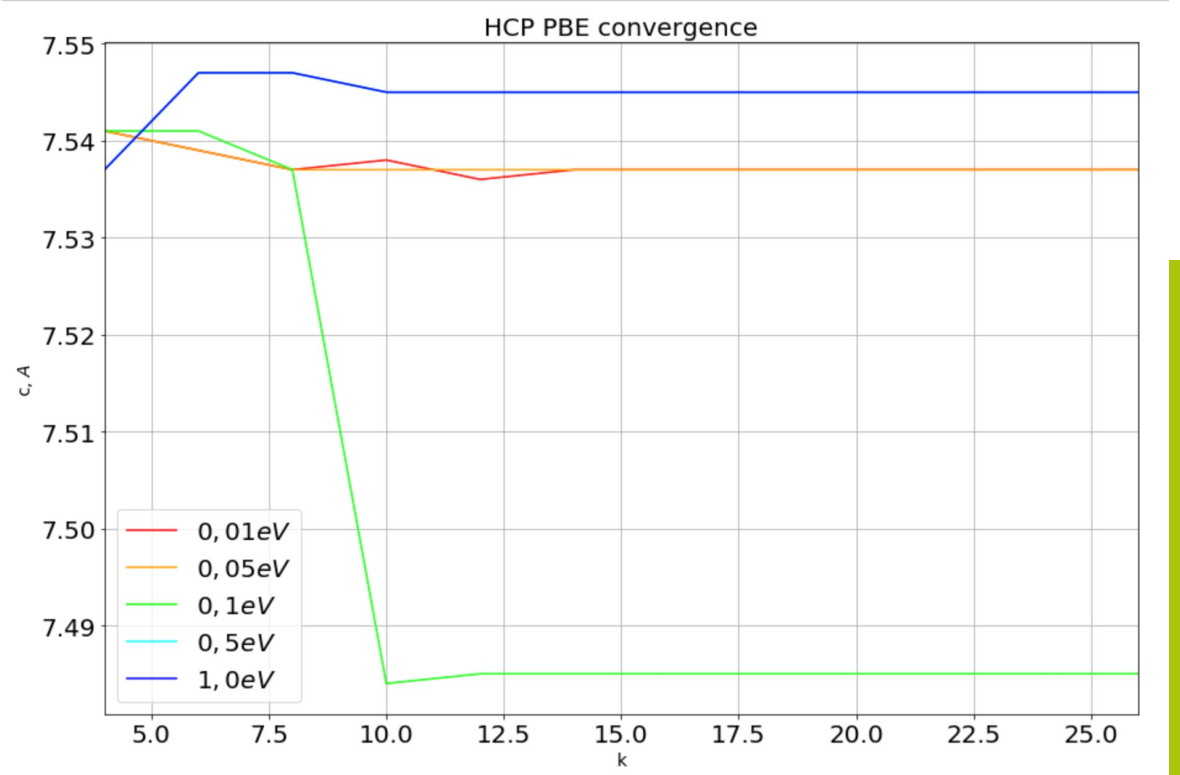


a_{exp}=6.695 A

μ=1.74 μ_B

ABINIT results.
Parameters convergence w/ respect to k-point mesh
HCP





a_{exp}=4.73 A

c_{exp}=7.667 A

μ= 2.000 $\forall k$ for smearing = 0.01eV, 0.05 eV;

μ= 2.000 for k<=10 for smearing 0.1 eV, μ= 0.000 for k > 10

μ= 0.000 2.000 $\forall k$ for smearing = 0.5 eV, 1.0 eV

$\mu_{exp} = 1.72$

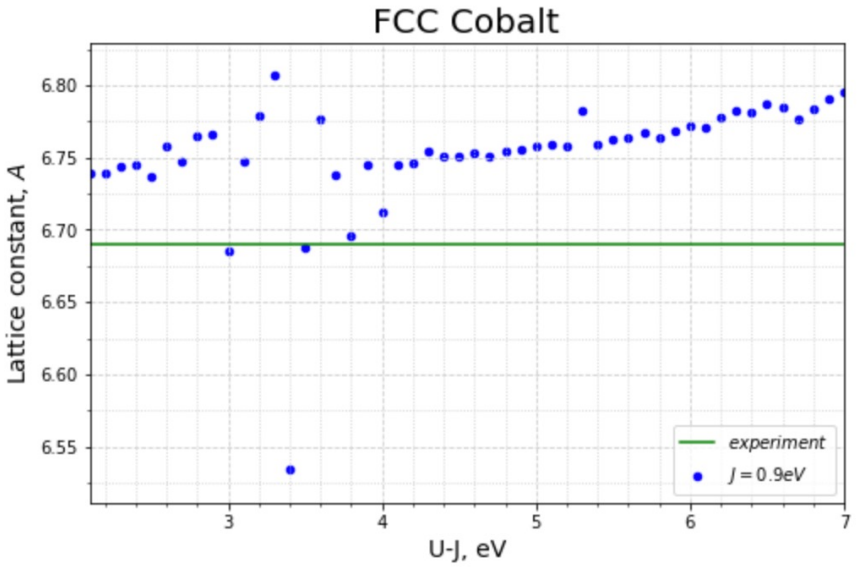
ABINIT. DFT+U. Preliminary research.

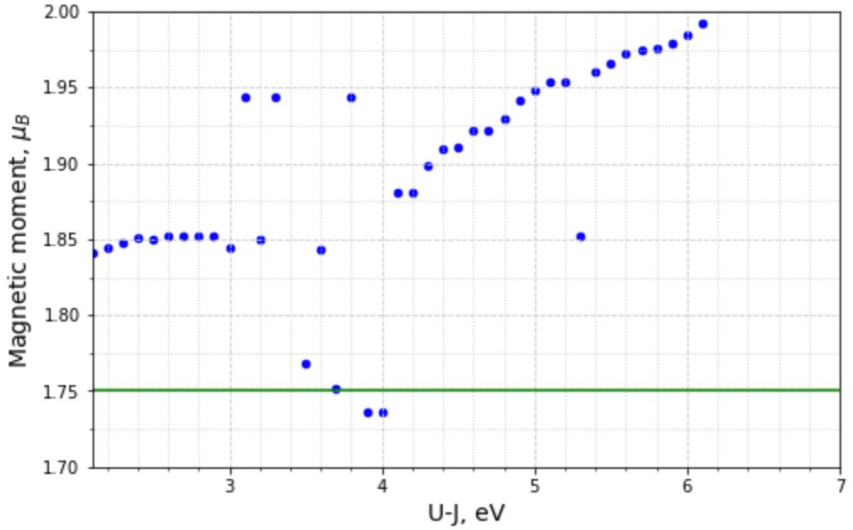
Paper	U_{eff},eV	U, eV	J, eV
Korotin, M. A., Ezhov, S. Y., Solovyev, I. V., Anisimov, V. I., Khomskii, D. I., & Sawatzky, G. A. (1996). Intermediate-spin state and properties of **LaCoO 3**. *Physical Review B*, *54*(8), 5309.	6.88	7.8	0.92
Wdowik, U. D., & Parlinski, K. (2009). Lattice dynamics of Fe-doped **CoO** from first principles. *Journal of Physics: Condensed Matter*, *21*(12), 125601.	6.1	-	-
Wang, H., Yan, Y., Mohammed, Y. S., Du, X., Li, K., & Jin, H. (2009). The role of Co impurities and oxygen vacancies in the ferromagnetism of **Co-doped SnO2**: GGA and GGA+ U studies. *Journal of magnetism and magnetic materials*, *321*(19), 3114-3119.	4.08	-	-
Mohammed, Y. S., Yan, Y., Wang, H., Li, K., & Du, X. (2010). Stability of ferromagnetism in Fe, **Co**, and ni metals under high pressure with GGA and GGA+ U. *Journal of magnetism and magnetic materials*, *322*(6), 653-657.	2.4	-	-
Vega, A., & Nolting, W. (1996). Finite-temperature ferromagnetism of **fcc cobalt**. *physica status solidi (b)*, *193*(1), 177-187.	3.2	-	-
Illas, F. (2010). Electronic and magnetic structure of **bulk cobalt**: The, and ε-phases from density functional theory calculations. *The Journal of chemical physics*, *133*, 024701.	3.0	-	-
Cococcioni, M., & De Gironcoli, S. (2005). Linear response approach to the calculation of the effective interaction parameters in the LDA+ U method. *Physical Review B*, *71*(3), 035105.			

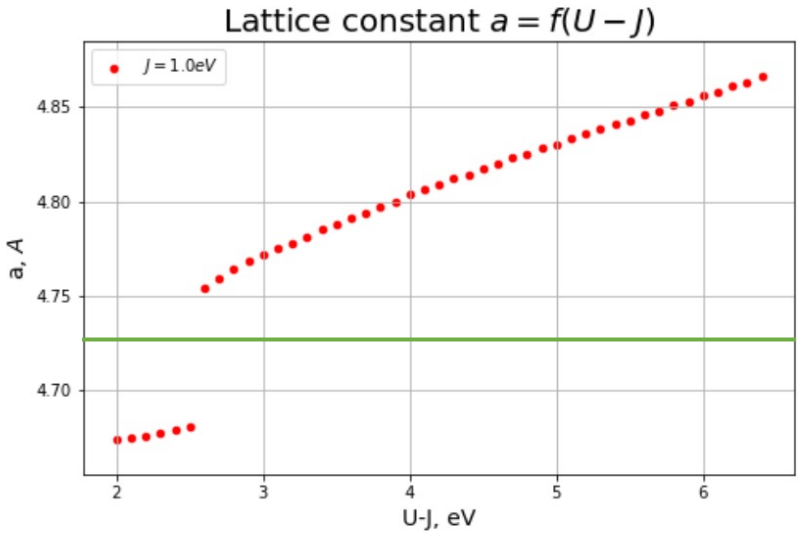
ABINIT results. DFT+U

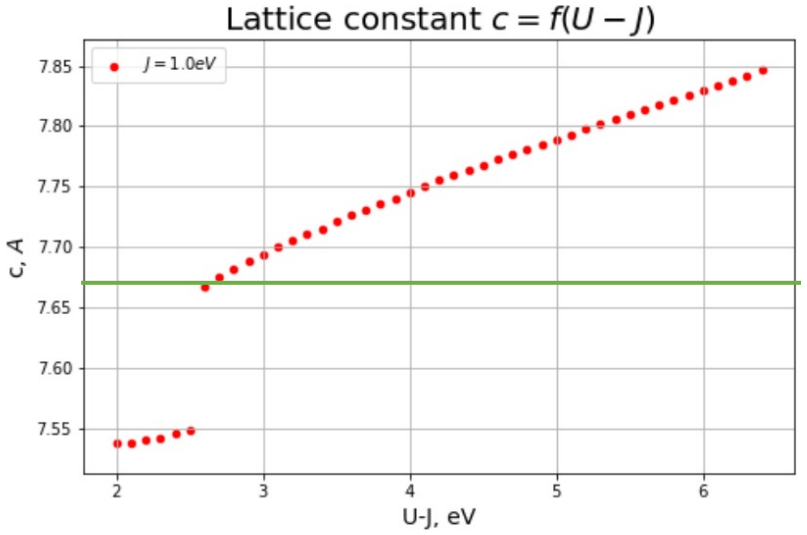
HCP Cobalt

$\mu \sim$ 2.000 everywhere



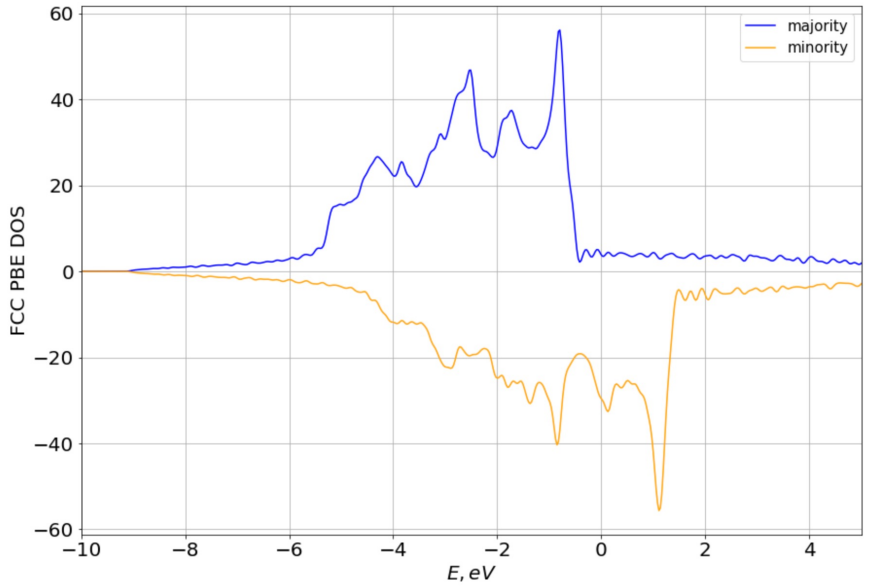


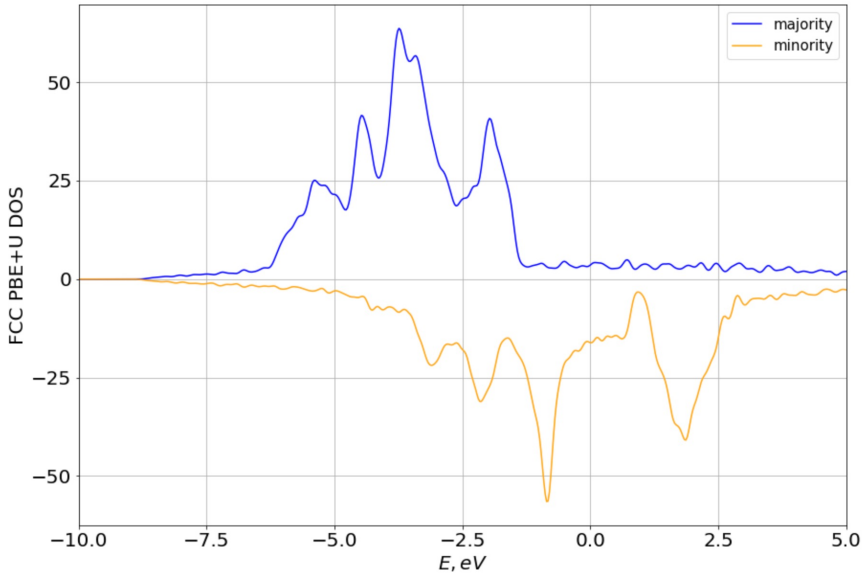




ABINIT results. DOS. FCC

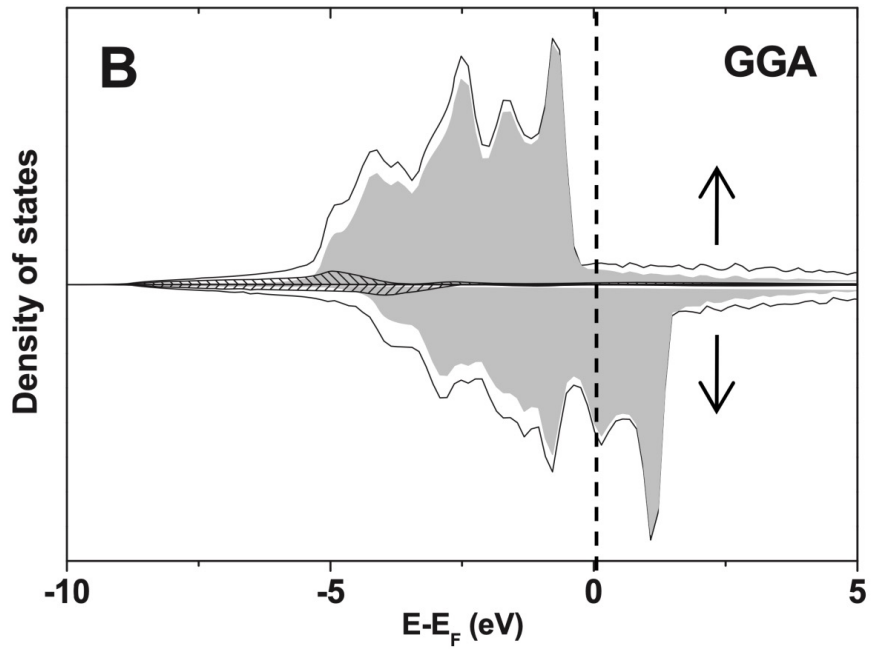
Illas, F. (2010). Electronic and magnetic structure of bulk cobalt: The, and ε-phases from density functional theory calculations. *The Journal of chemical physics*, *133*, 024701.

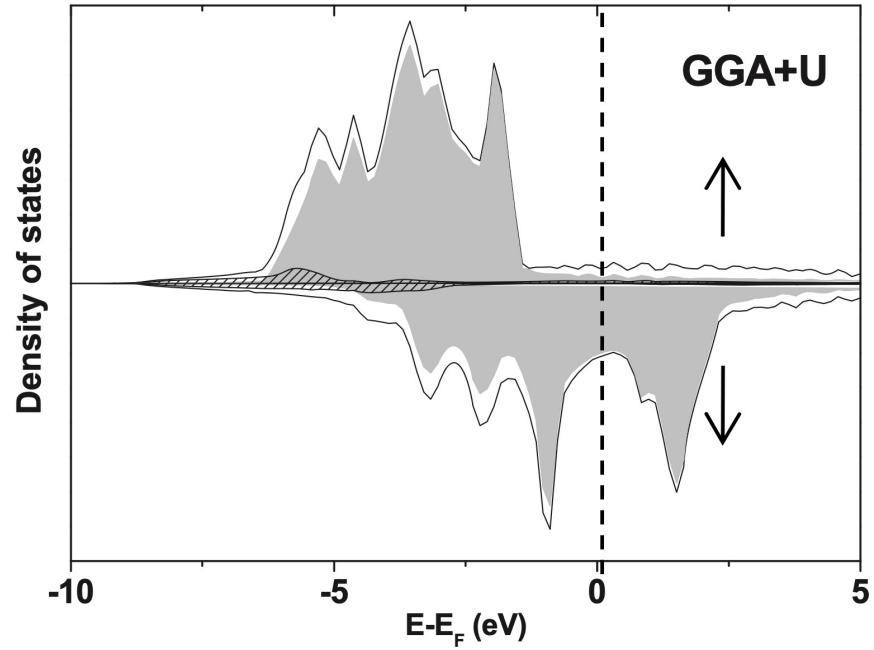




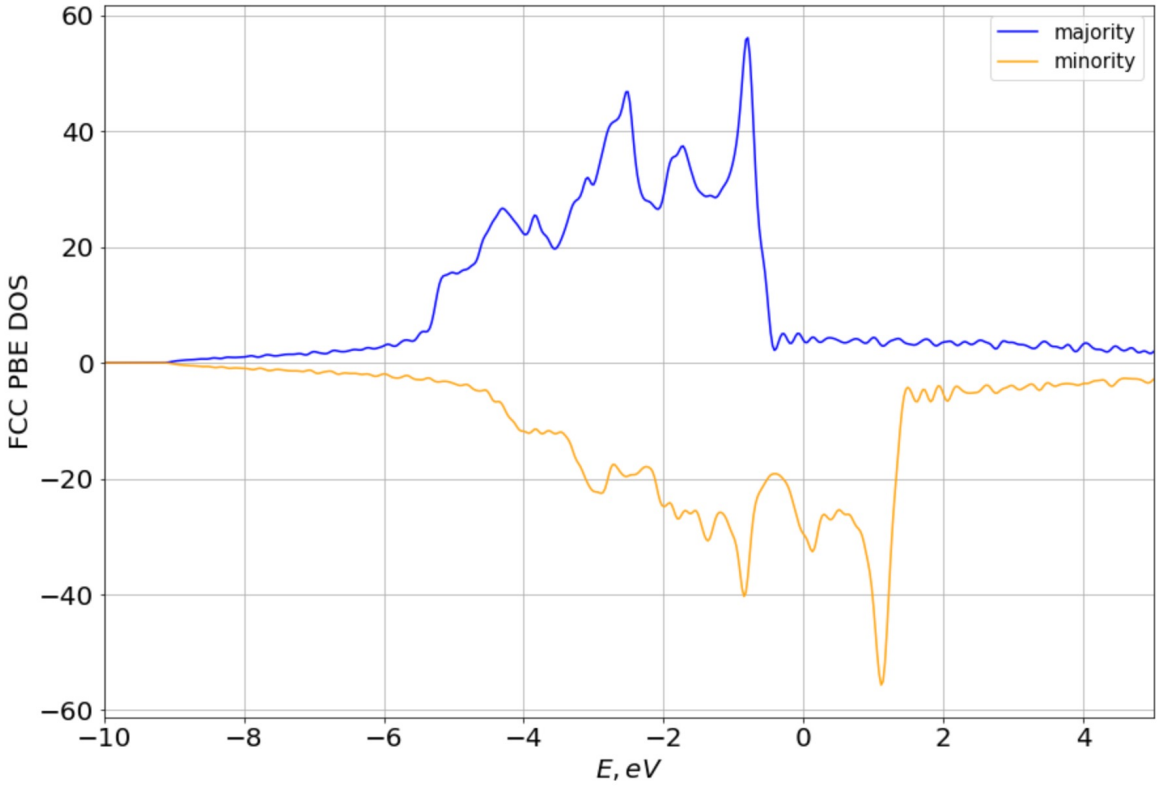
U=4.0 eV

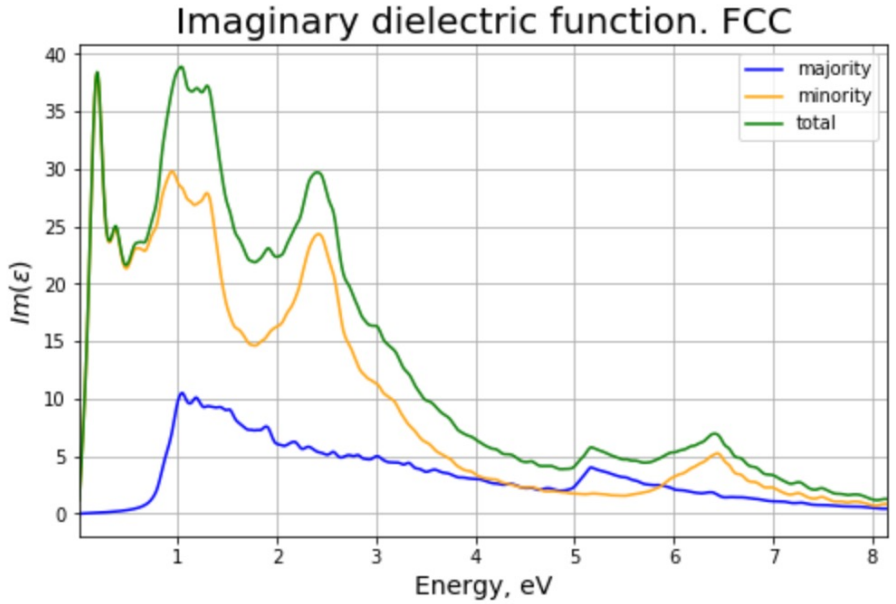
J=1.0 eV

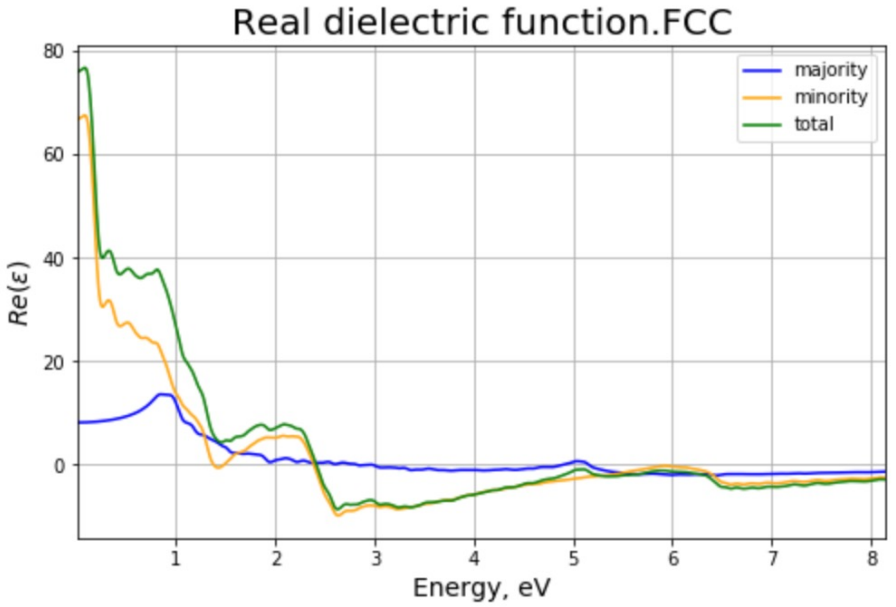




ABINIT results. Dielectric function. FCC

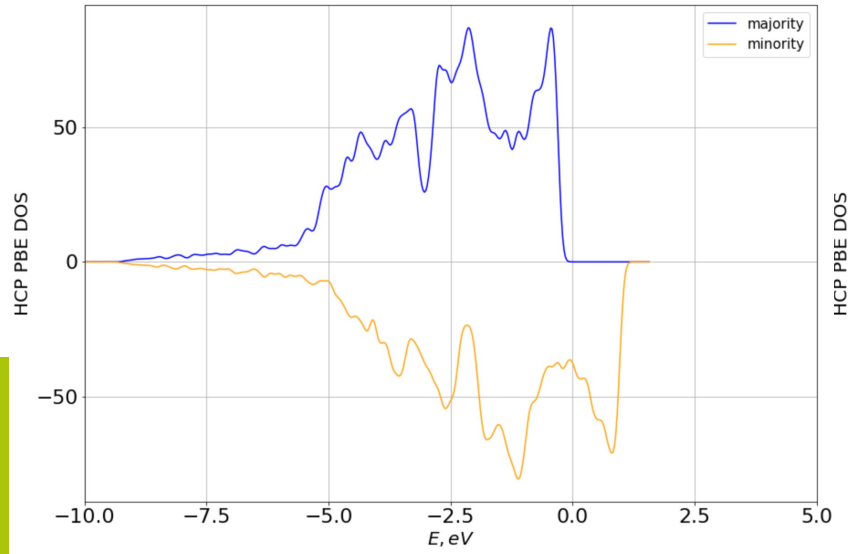


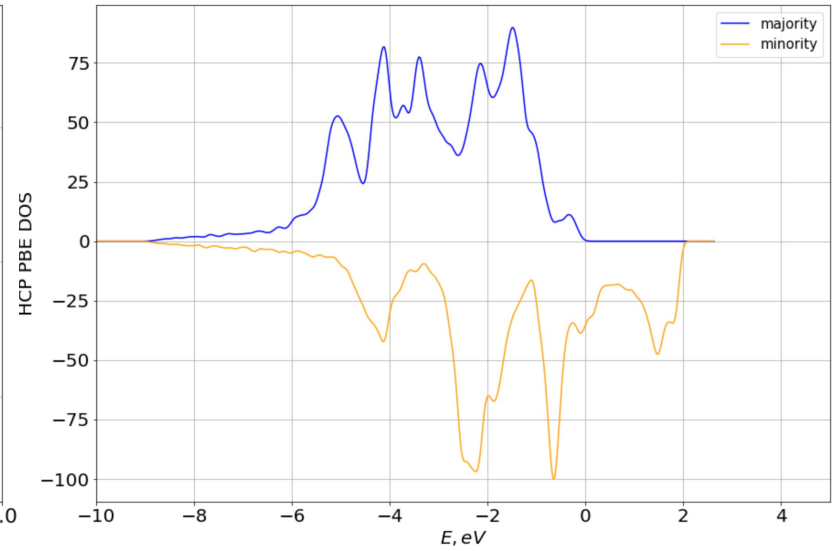




ABINIT results. DOS. HCP

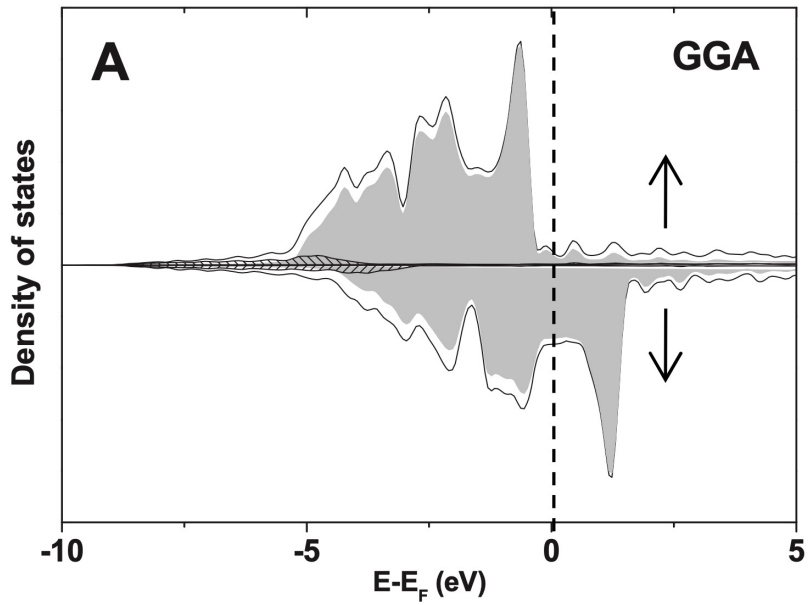
Illas, F. (2010). Electronic and magnetic structure of bulk cobalt: The, and ε-phases from density functional theory calculations. *The Journal of chemical physics*, *133*, 024701.

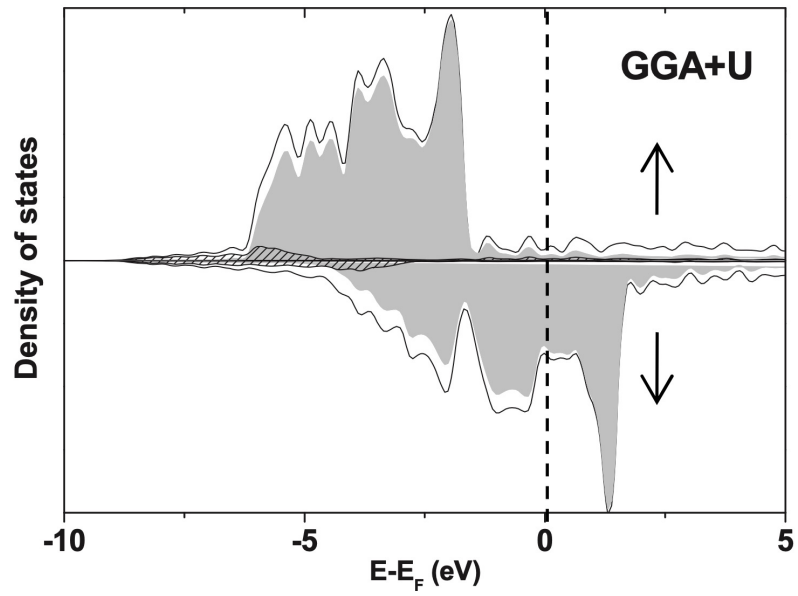




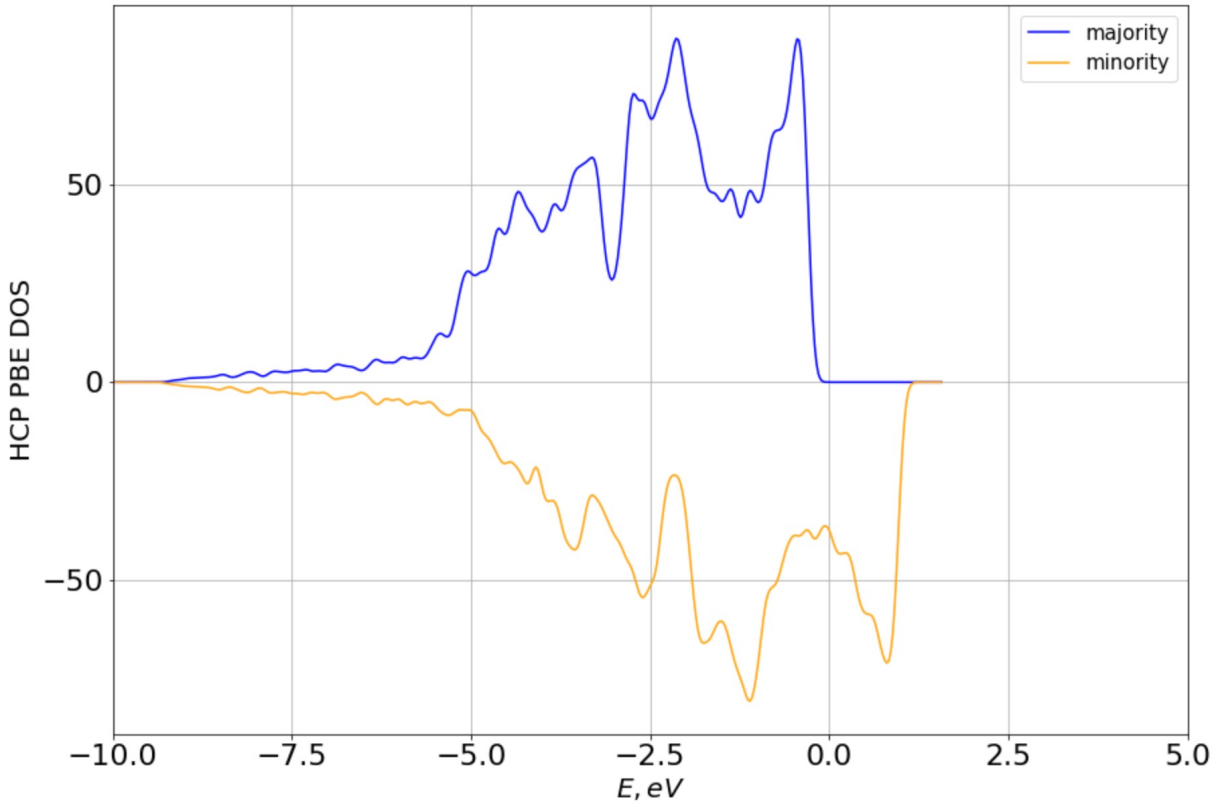
U=4.0 eV

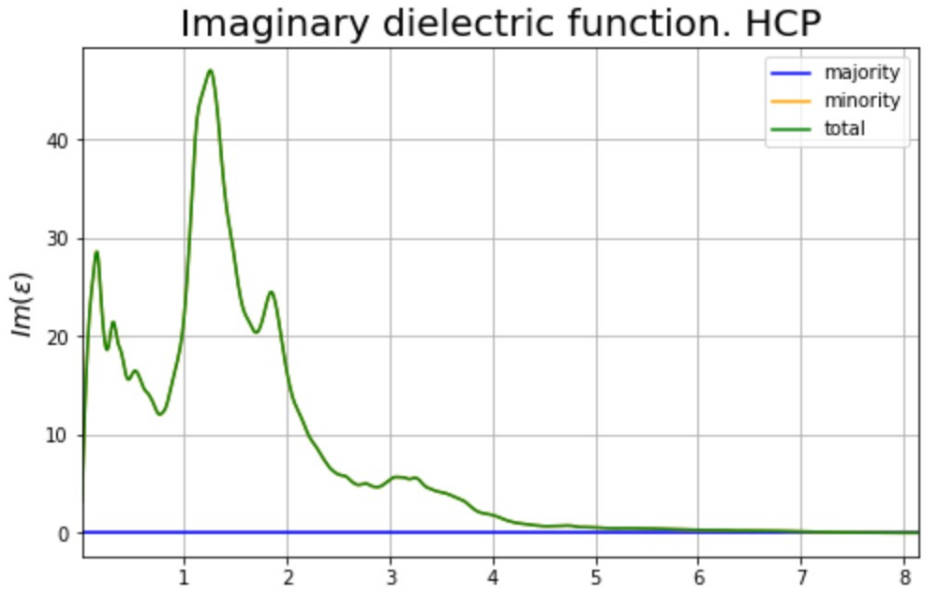
J=1.0 eV

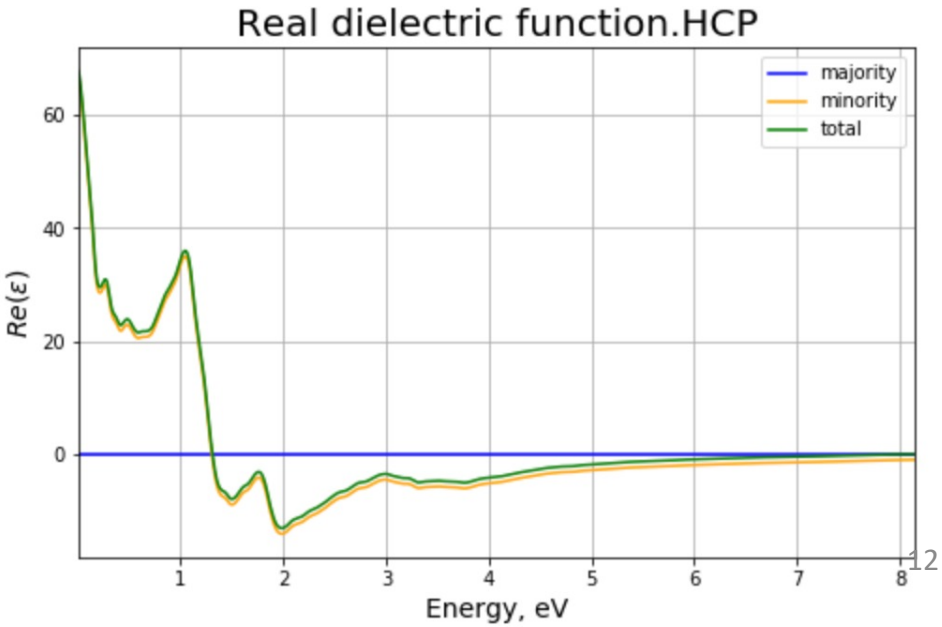




ABINIT results. Dielectric function. HCP





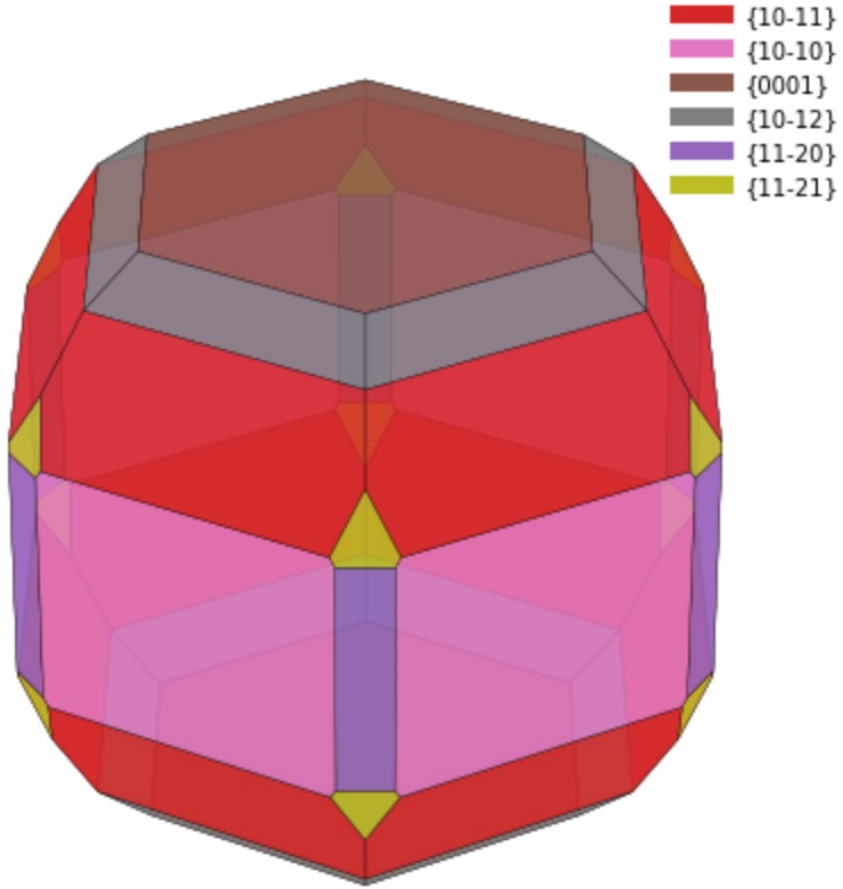


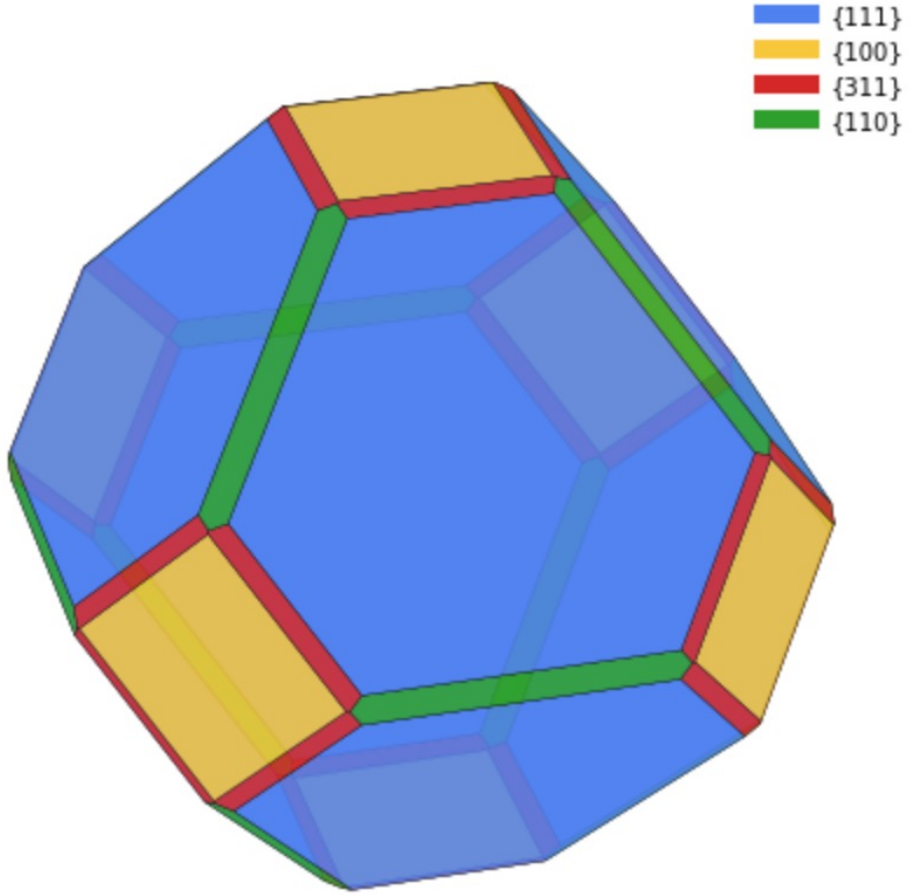
FHI-aims

Clusters. Wulff construction

J. M. Rahm and P. Erhart
Journal of Open Source Software **45**, 1944 (2020)

$$\min_i \Delta G_i = \min_j \sum_j \gamma_j S_j$$



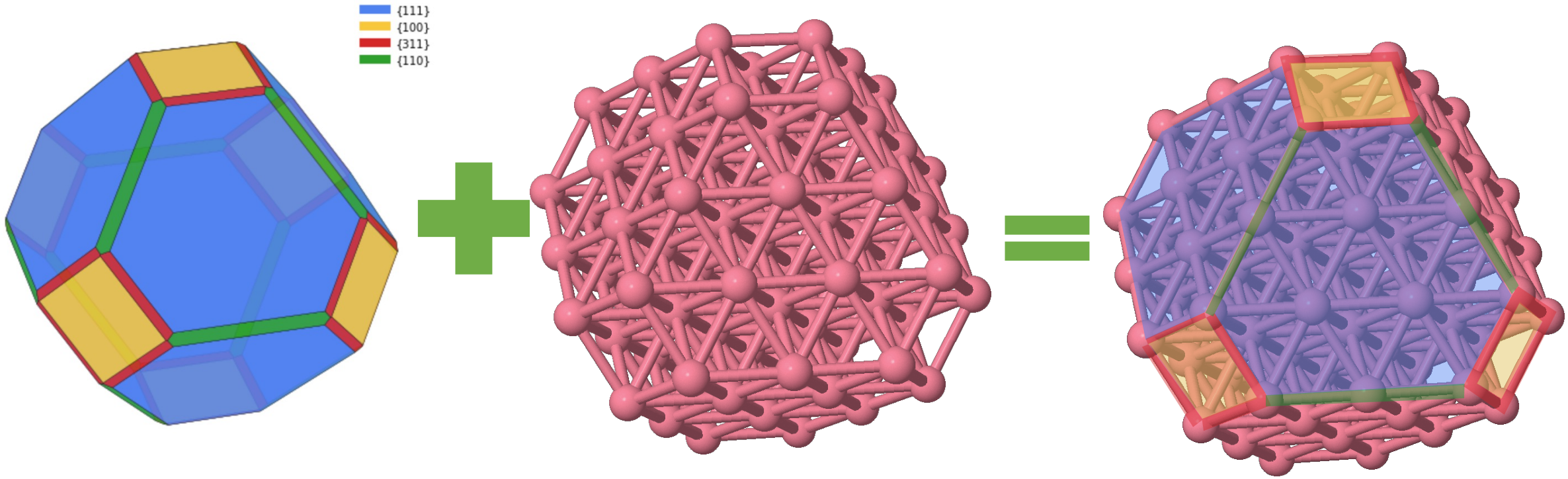


Liu J. X. et al. Crystallographic dependence of CO activation on cobalt catalysts: HCP versus FCC //Journal of the American Chemical Society. – 2013. – Т. 135. – №. 44. – С. 16284-16287.

FCC cluster

79 atoms

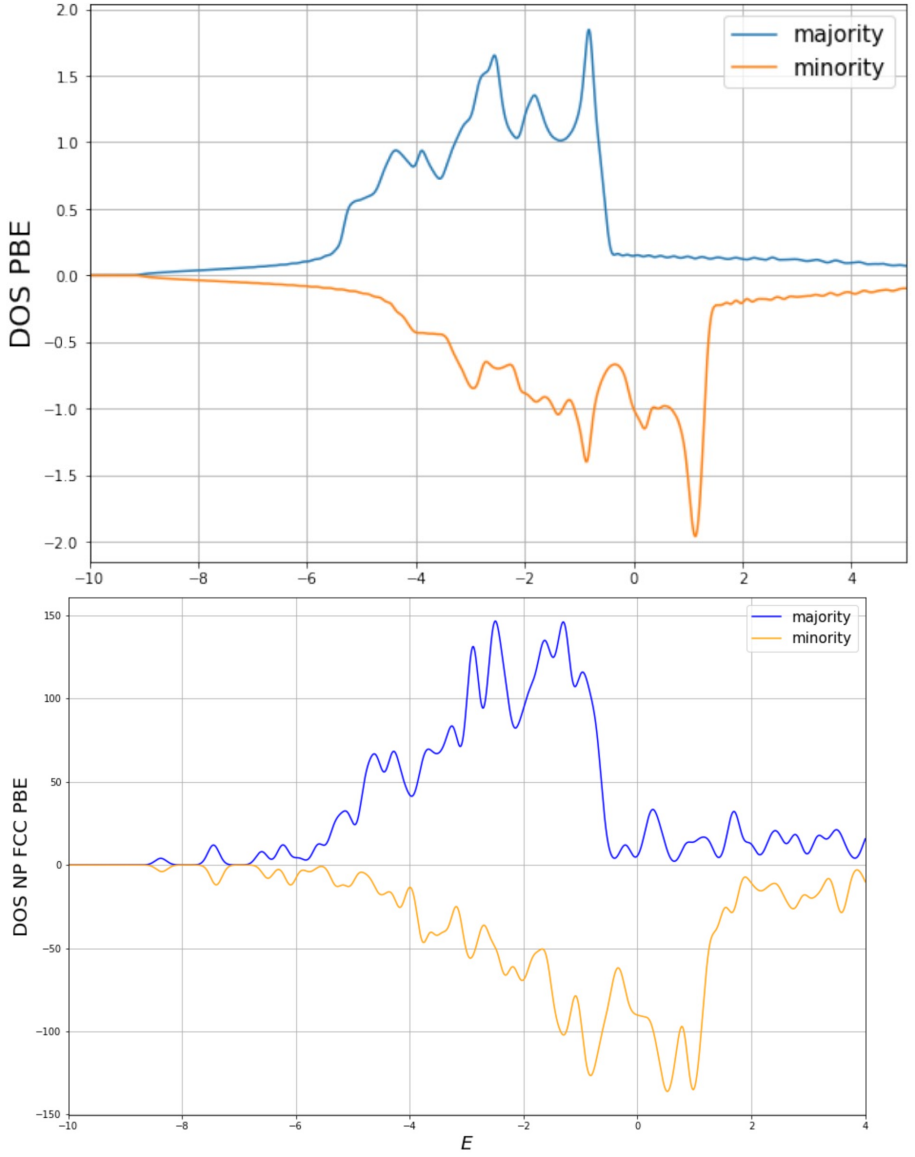
μ=1.74



For bulk FCC Cobalt lattice constant a=3.522 A

In relaxed cluster interatomic distances vary from 2.36 to 2.49 A (less on the surface, more in the center)

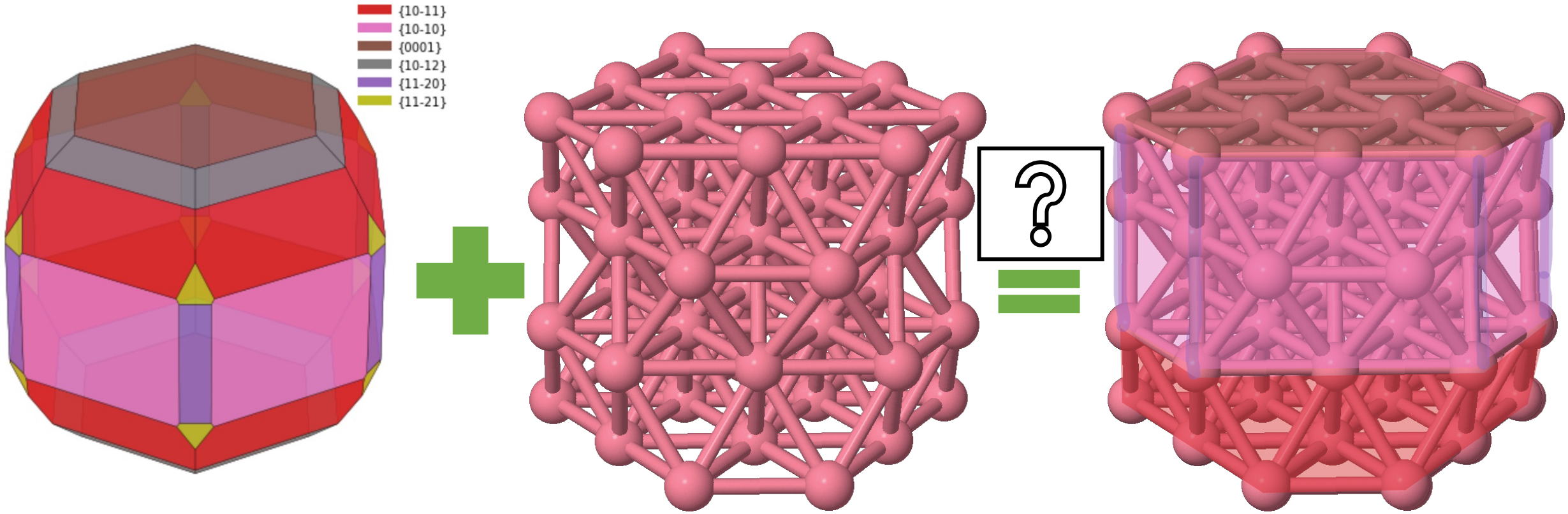
FCC cluster. DOS comparison



HCP cluster

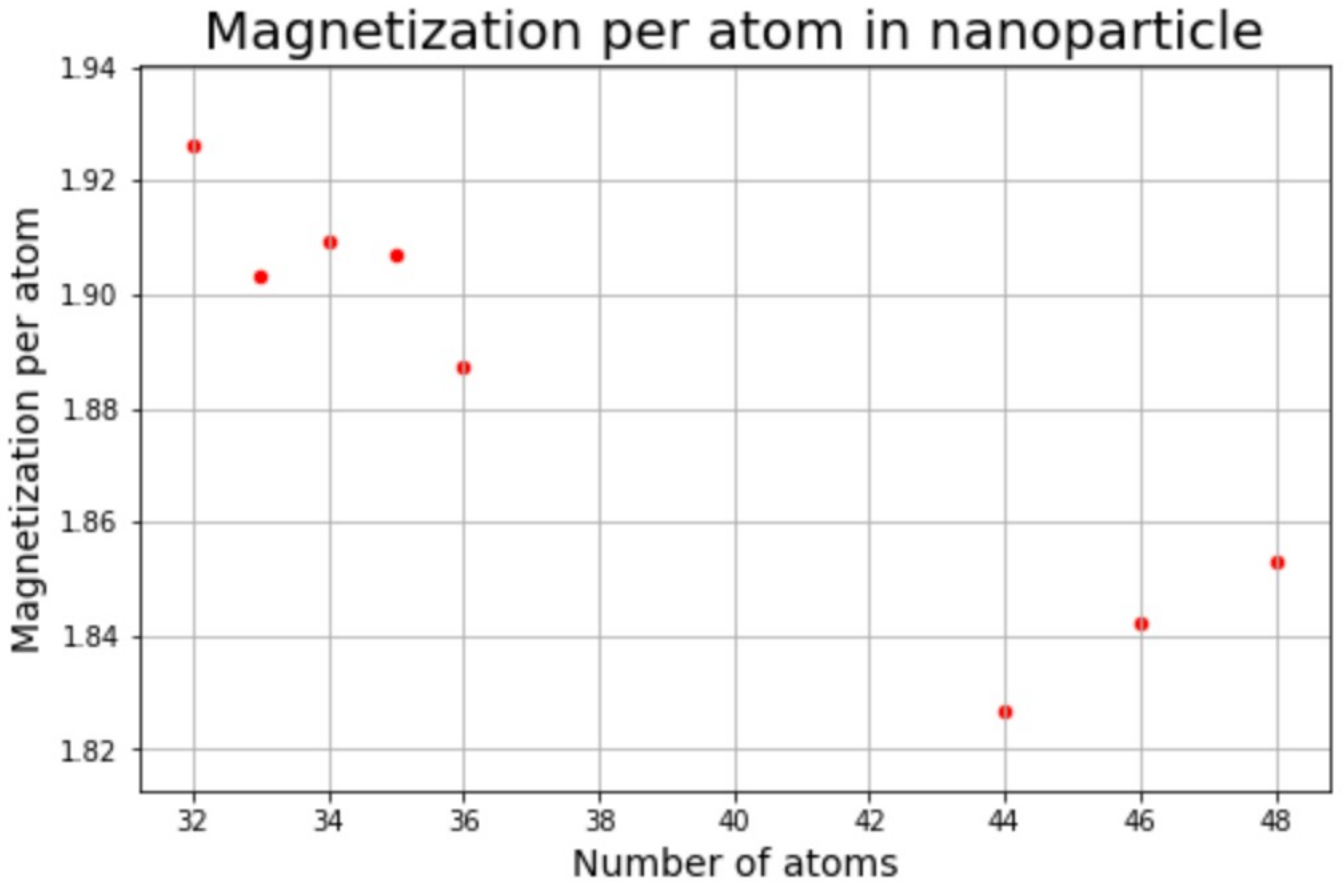
48 atoms

μ= 1.85



Bulk: a = 2.501 A, c = 4.033 A

Cluster: a = [2.36A, 2.49]; c= [3.92 A, 3.99A]



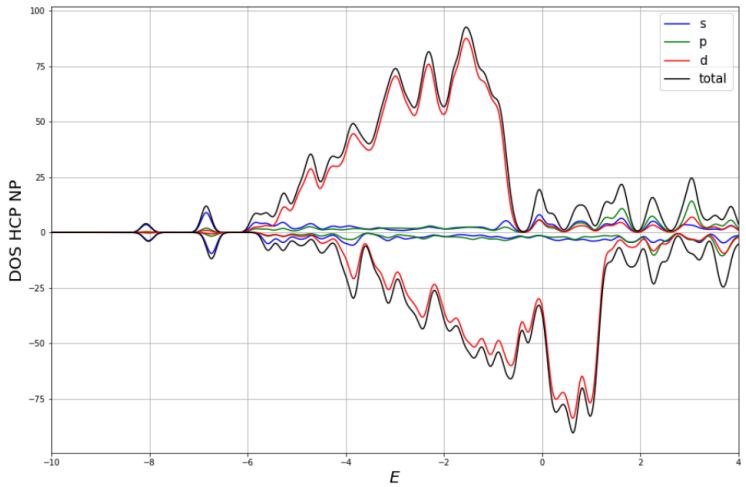
Use molecular dynamics

Use evolutionary algorithm (USPEX) to find the optimal shape of a cluster w/ fixed number of atoms

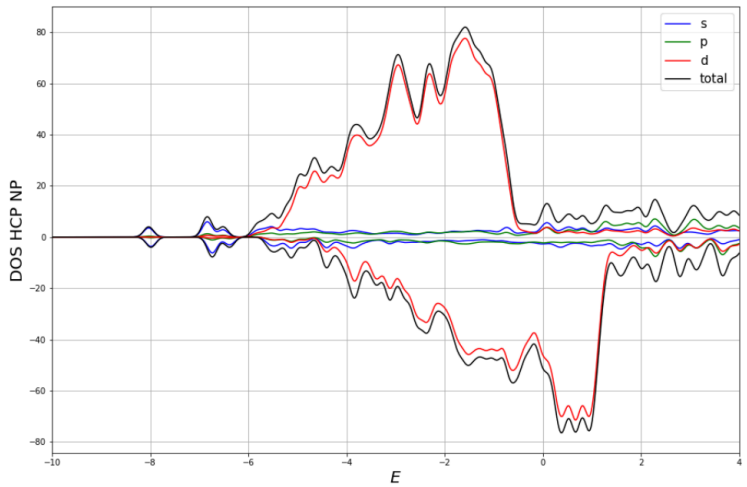
Check dependence on the spin orientation

HCP cluster. DOS comparison

48



44



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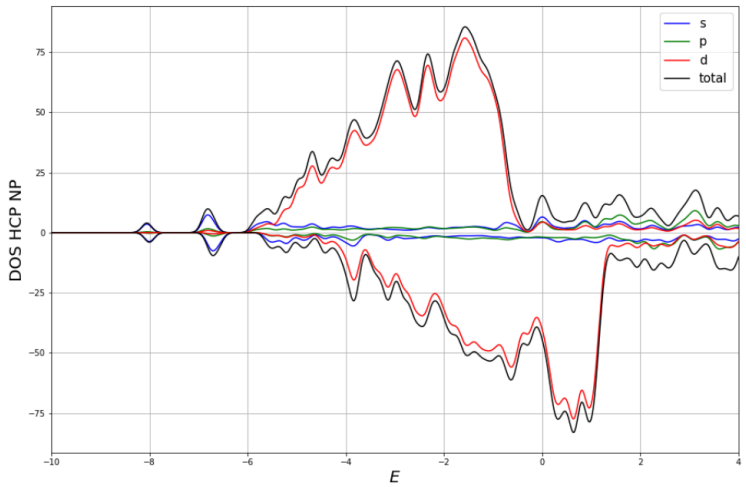
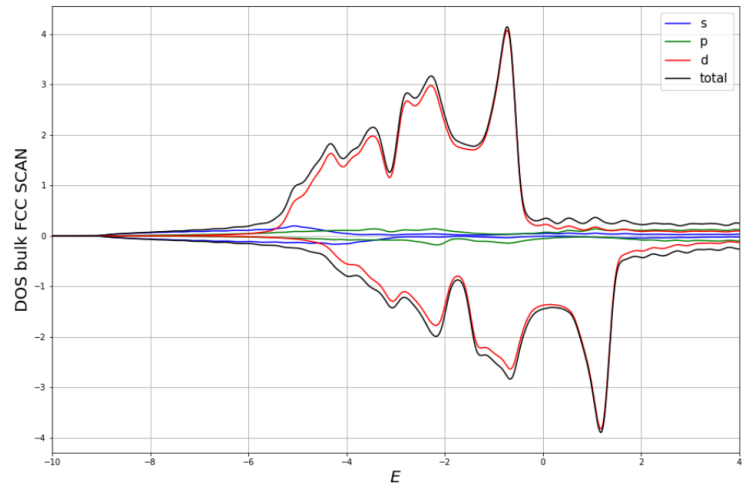


bulk



Thank you!