TO WHAT EXTENT DO CHEMICAL DESCRIPTORS BEHAVE AS SUCH?

STUDY OF ELECTRONIC CHEMICAL DESCRIPTORS FOR HCP TRANSITION METALS

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OBJECTIVES

12 HCP TRANSITION METALS:

Sc, Y, Ti, Zr, Hf, Tc, Re, Ru, Os, Co, Zn and Cd.

3 SURFACES:

(0001), $(10\bar{1}0)$, and $(11\bar{2}0)$

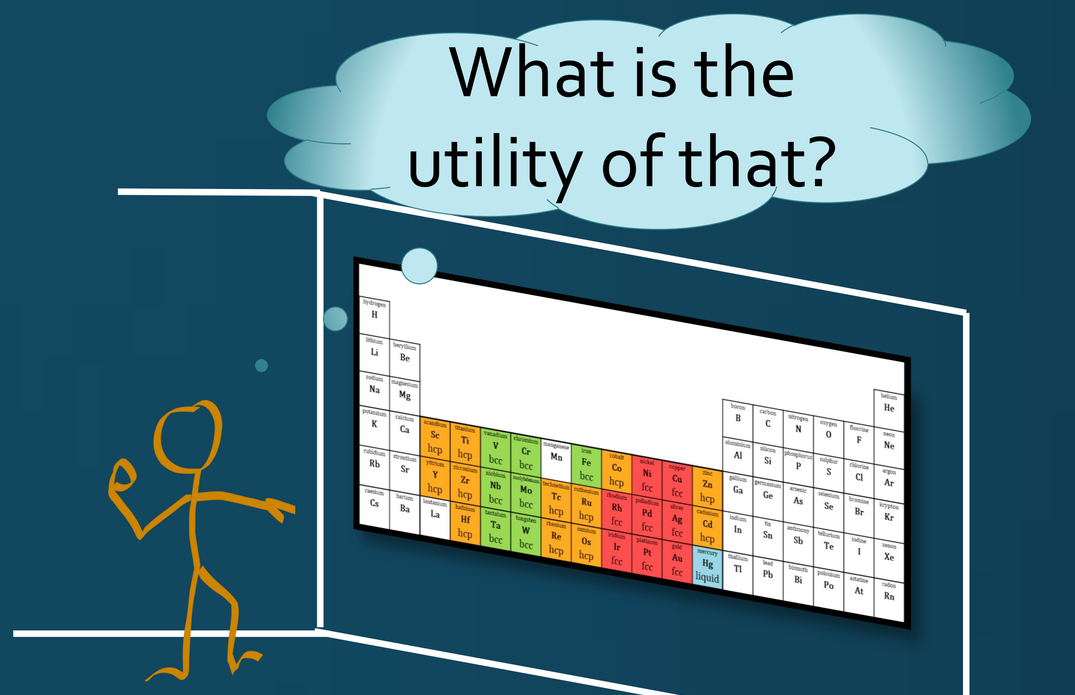
2 FUNCTIONALS:

PBE and TPSS

Simulate isolated atoms and bulks → Cohesive energies

Simulate surfaces → Surface Energies, Relaxation energies

To obtain and analyze three chemical descriptors → *d*-band center; Width corrected *d*-band center; Maximum point of the Hilbert transform of the *d*-band



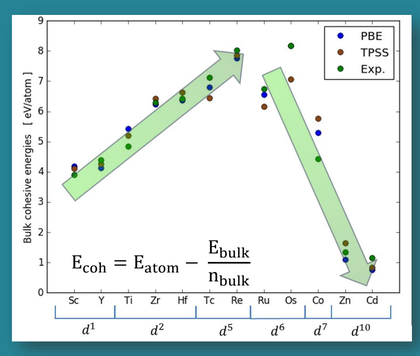
- Knowing a descriptor value one can predict the activity of metallic surface in an easier way than simulating the process.
  - An study of the hcp transition metals allows studying possible periodic trends as they are distributed all along the periodic table.

What is a descriptor?

A parameter that follows the trends of a property, but is easier to calculate.

BULK COHESIVE ENERGY

Cohesive energy describes how much stable is the bulk in front of the isolated atoms. The higher is the cohesive energy, the more stable is the bulk.



The bulk cohesive energies follow a volcano shape structure.

	E_{coh}				δ			
	PBE		TPSS		PBE		TPSS	
	Prev.	Exp.	Prev.	Exp.	Prev.	Exp.	Prev.	Exp.
MPE	-0.2	-5.2	-5.0	-1.9	-1.2	-1.4	0.0	-2.4
MAPE	1.1	10.9	8.7	11.6	1.5	2.3	1.5	3.5

Broken bond model not followed.

Relative stability of surfaces:

(0001) < $(11\bar{2}0)$ < $(10\bar{1}0)$

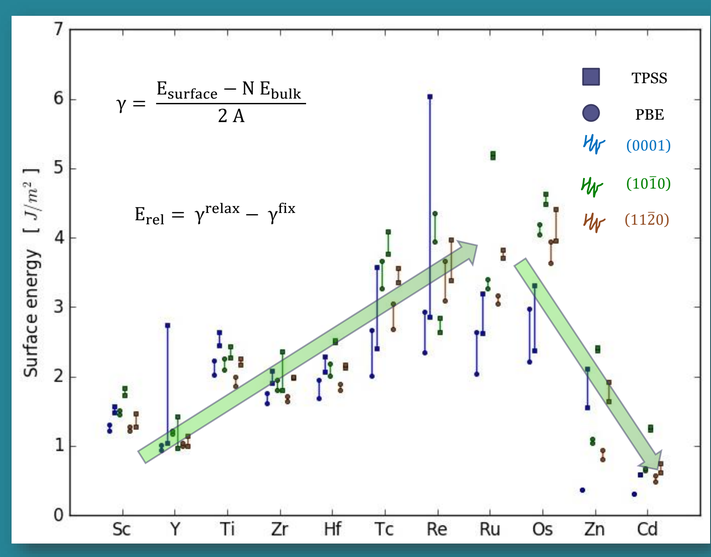
CN = 9 CN = 7 CN = 8

Same volcano shape seen in cohesive energies.

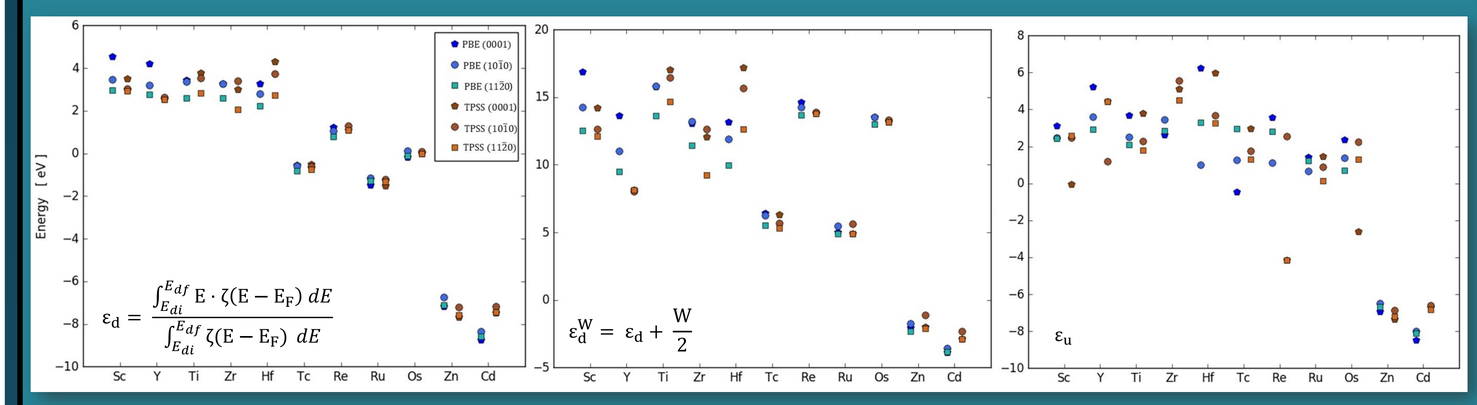
Higher relaxation energies in unstable surfaces.

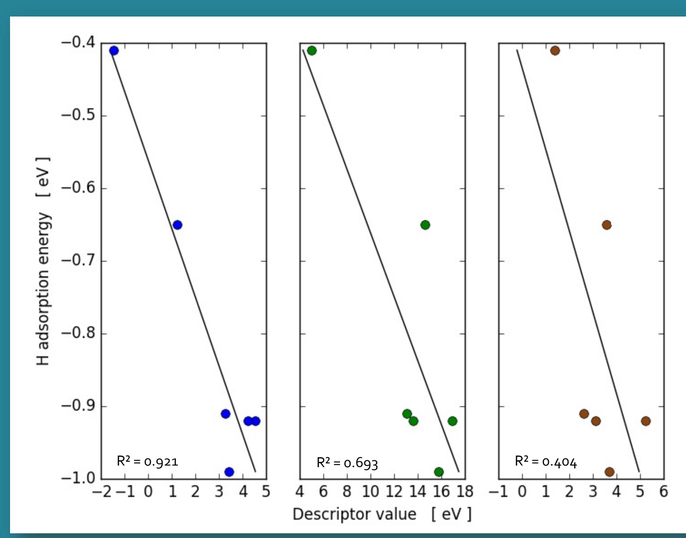
SURFACE ENERGY

Surface energy describes how much unstable is to have a surface instead of having a bulk structure.

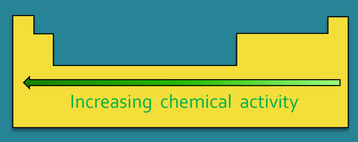


CHEMICAL DESCRIPTORS RESULTS



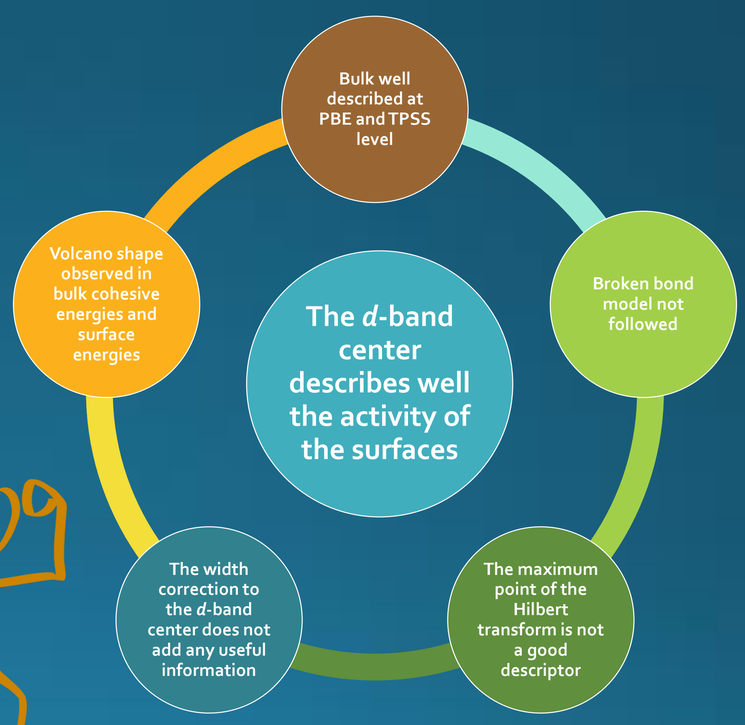


- Checking hydrogen adsorption energies the trend of the chemical activity is seen to be:



- ε_d is the descriptor that fits better the hydrogen adsorption energies.
- ε_d^W and ε_u fitting is worse, having also a bad qualitative description of the activity trend.

CONCLUSIONS



References:

1. *J. Chem. Theory Comput.* **2013**, 9, 1631–1640.
2. *J. Chem. Theory Comput.* **2014**, 10, 3832–3839.
3. *Surf. Sci.* **2012**, 606, 1400-1404