BCC TRANSITION METAL SURFACES: TRENDS IN WORK FUNCTIONS AND SURFACE ENERGIES

Lorena Vega, Francesc Viñes

Department de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTC), Facultat de Química i Física, C/Martí i Franqués, 1 (08028) Barcelona

Email: vegalorena24@gmail.com

MOTIVATION

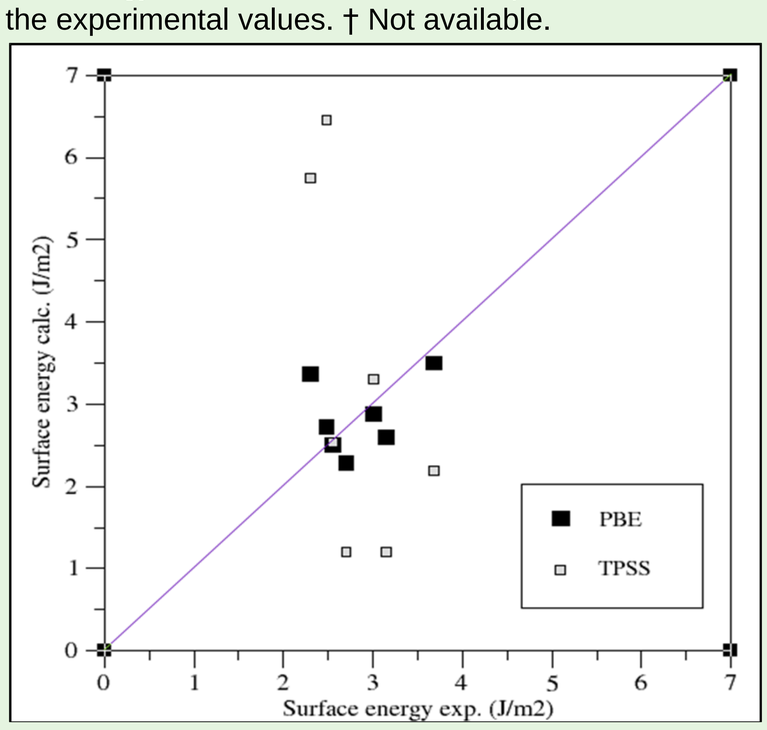
- Ascertain the accuracy of PBE and TPSS in describing surface stability and relaxation.
- Inspect the possible correlation of surface stability with the packing degree and bulk cohesive energy.
- Assess the accuracy of PBE and TPSS in estimating ϕ values, comprehend the trends of it with respect periodic table series and groups, and rationalize the ϕ variation from one surface ending to another.

RESULTS

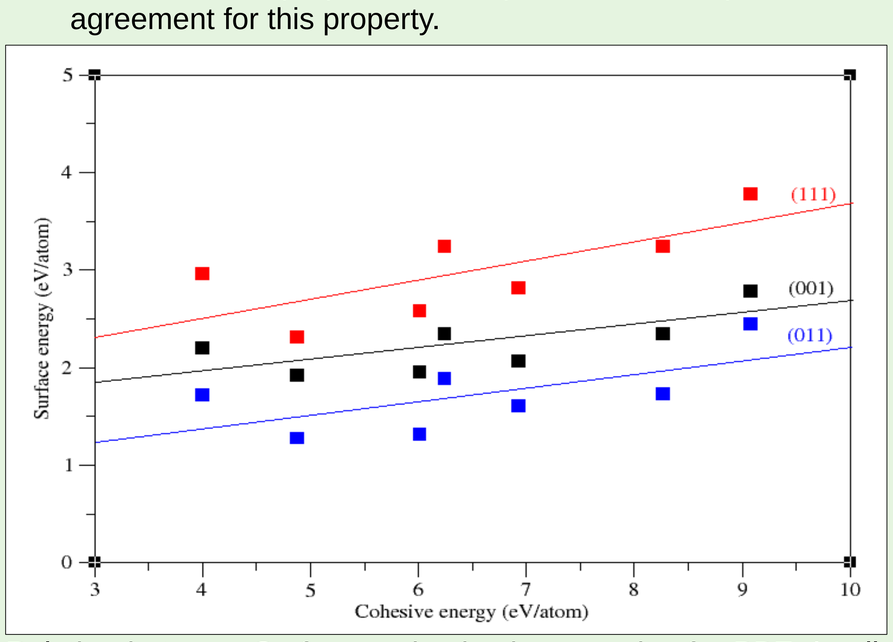
SURFACE ENERGY

Metal	PBE (001)	PBE (011)	PBE (111)	PBE $\bar{\gamma}$	TPSS (001)	TPSS (011)	TPSS (111)	TPSS $\bar{\gamma}$	Exp.
V	2.39	2.41	2.70	2.50	2.62	0.35	4.66	2.54	2.55
Nb	2.35	2.14	2.36	2.28	1.26	0.42	1.92	1.20	2.70
Ta	2.51	2.56	2.72	2.60	1.22	0.28	2.11	1.20	3.15
Cr	3.42	3.29	3.40	3.37	5.34	5.42	6.48	5.75	2.30
Mo	3.01	2.64	2.98	2.88	3.45	3.01	3.44	3.30	3.00
W	3.89	3.14	3.47	3.50	1.57	†	2.80	2.19	3.68
Fe	2.57	2.93	2.67	2.72	5.32	8.79	5.24	6.45	2.48

Surface energy results, in J/m^2, and comparison between them and the experimental values. † Not available.

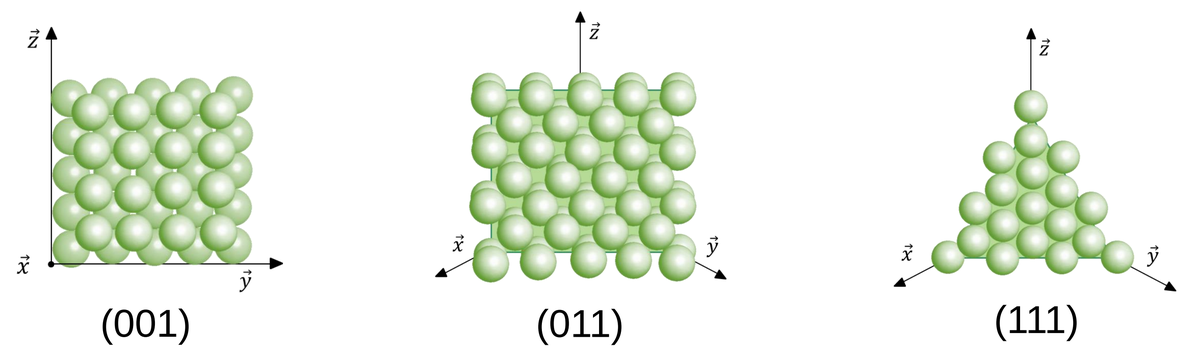


$\bar{\gamma}$ for TPSS and PBE levels against experimental values. The purple line represents the perfect agreement for this property.



Relation between Surface and cohesive energies for PBE. In all cases, the γ increases with E_{coh} with apparently a linear trend.

SURFACES

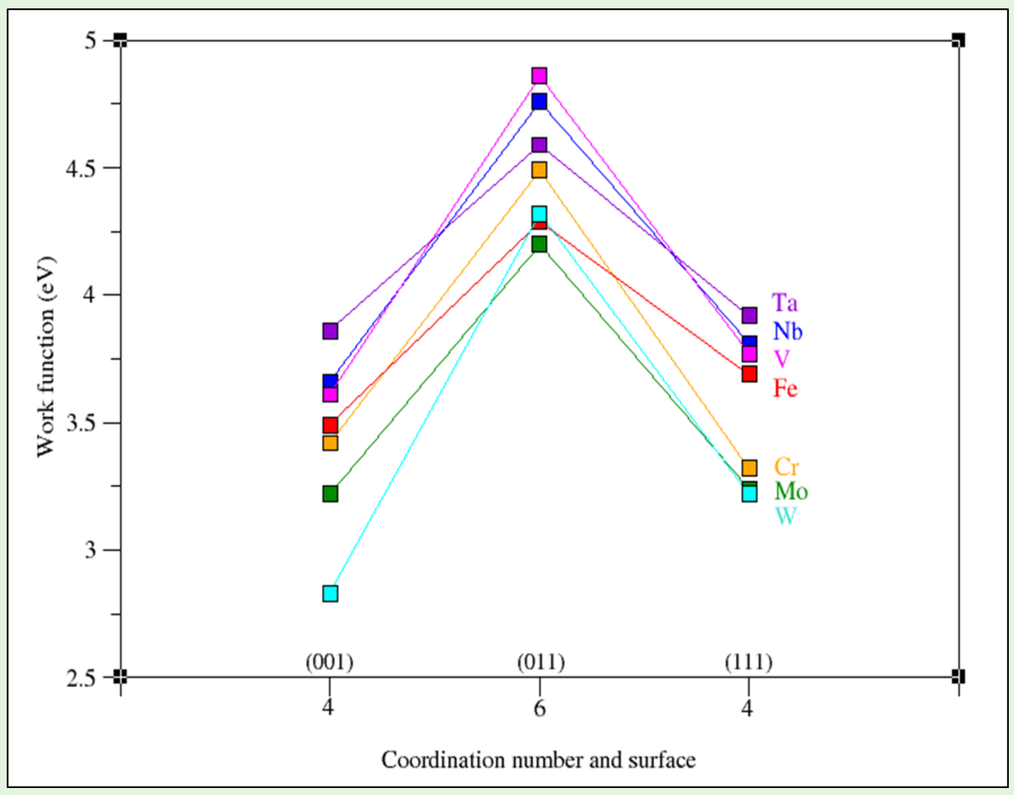


WORK FUNCTION

(001)			(011)			(111)		
V	Cr	Fe	V	Cr	Fe	V	Cr	Fe
4.30	4.50	4.50	4.30	4.50	4.50	4.30	4.50	4.50
2.83	3.66	3.61	4.32	4.76	4.86	3.22	3.81	3.77
4.38	4.29	4.52	3.90	5.15	6.94	3.75	3.72	4.02
Nb	Mo		Nb	Mo		Nb	Mo	
4.30	4.60		4.30	4.60		4.30	4.60	
3.22	3.49		4.20	4.29		3.24	3.69	
4.35	3.65		4.84	4.55		3.52	3.90	
Ta	W		Ta	W		Ta	W	
4.25	4.55		4.25	4.55		4.25	4.55	eV
3.42	3.86		4.49	4.59		3.32	3.92	
4.31	4.37		4.73	6.68		4.33	4.60	

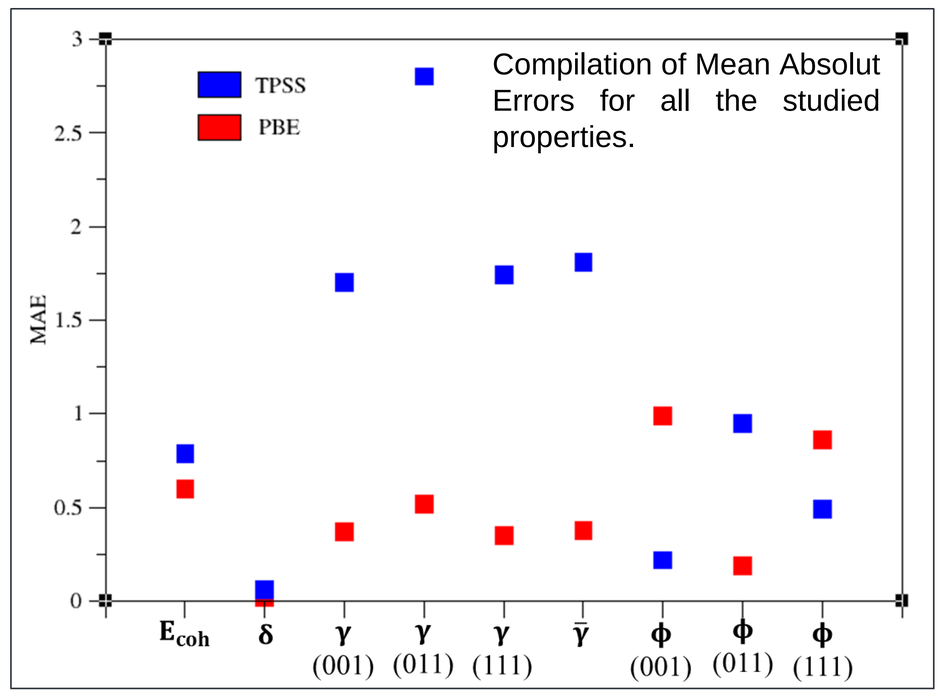
Exp. PBE TPSS

ϕ trend on series and groups. Red values are experimental data, black PBE values, and grey TPSS ones and relation between ϕ and CN of each surface on PBE (below).



CONCLUSIONS

- In general, **PBE gives less problems than TPSS**.
- An **increase** of the **coordination number** causes an increase of the surface stability because the **surface energy decreases**. Also cause an **increase of work function**.
- The **increase of the cohesive energy causes an increase of the surface energy.**
- This found relationships are general, but **not always strictly accomplished**.
- The work function **trend is clear in a series** but not on a group. The surface variation obtained is **ϕ(011)>ϕ(011)~ϕ(111),** which means (011) surface is the most stable one.



Compilation of Mean Absolut Errors for all the studied properties.

REFERENCES

1. Rosengaard, N. M., Skriver H. L. Surface energy and. Physical Review, **1992**, 46(11).
2. Owolabi, T. O., Akande, K. O., & Olatunji, S. O. . Support Vector Machines Approach for Estimating Work Function of Semiconductors: Addressing the Limitation of Metallic Plasma Model. Applied Physics Research, **2014**, 6(5), 122.