

Understanding the formation of Titania/MXene composites



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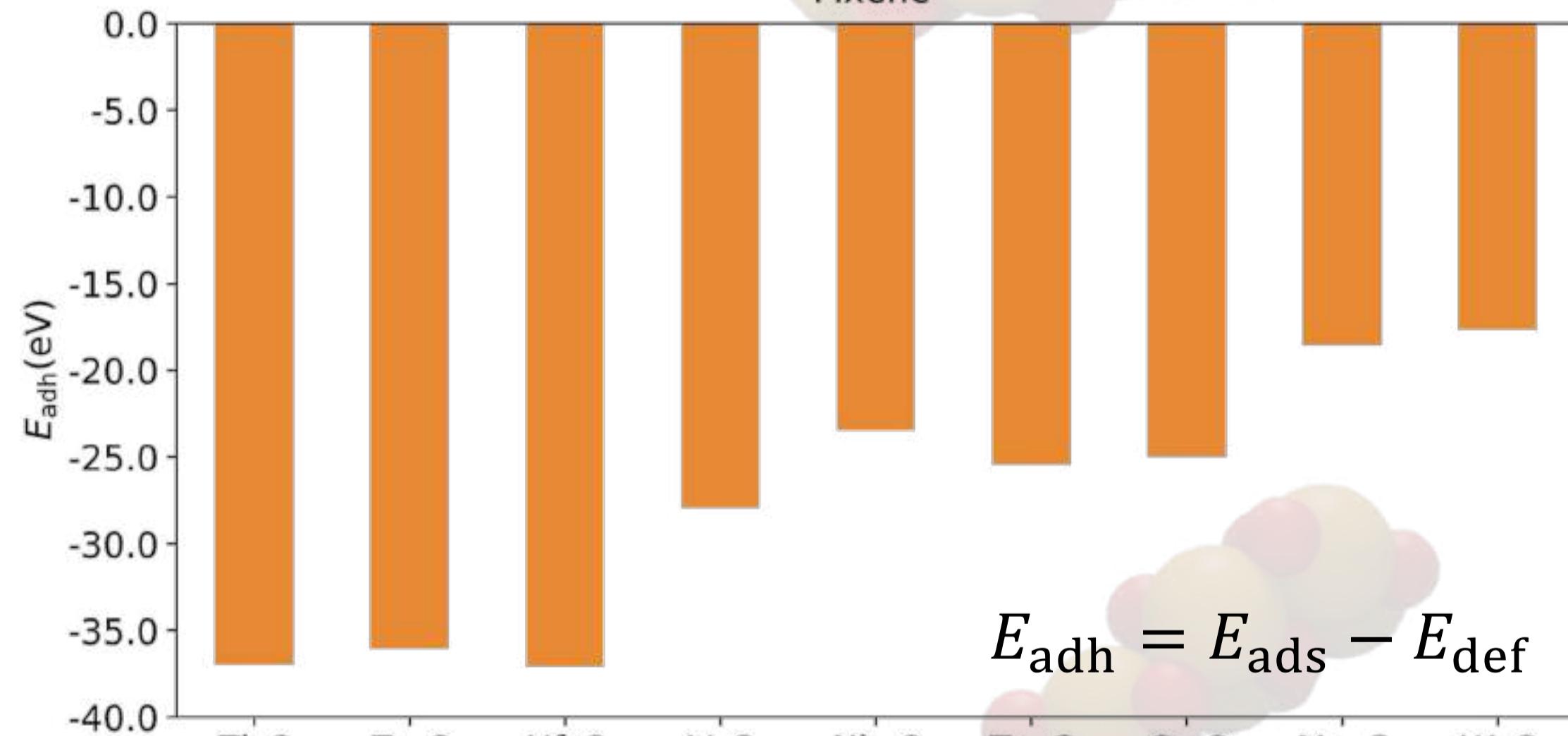
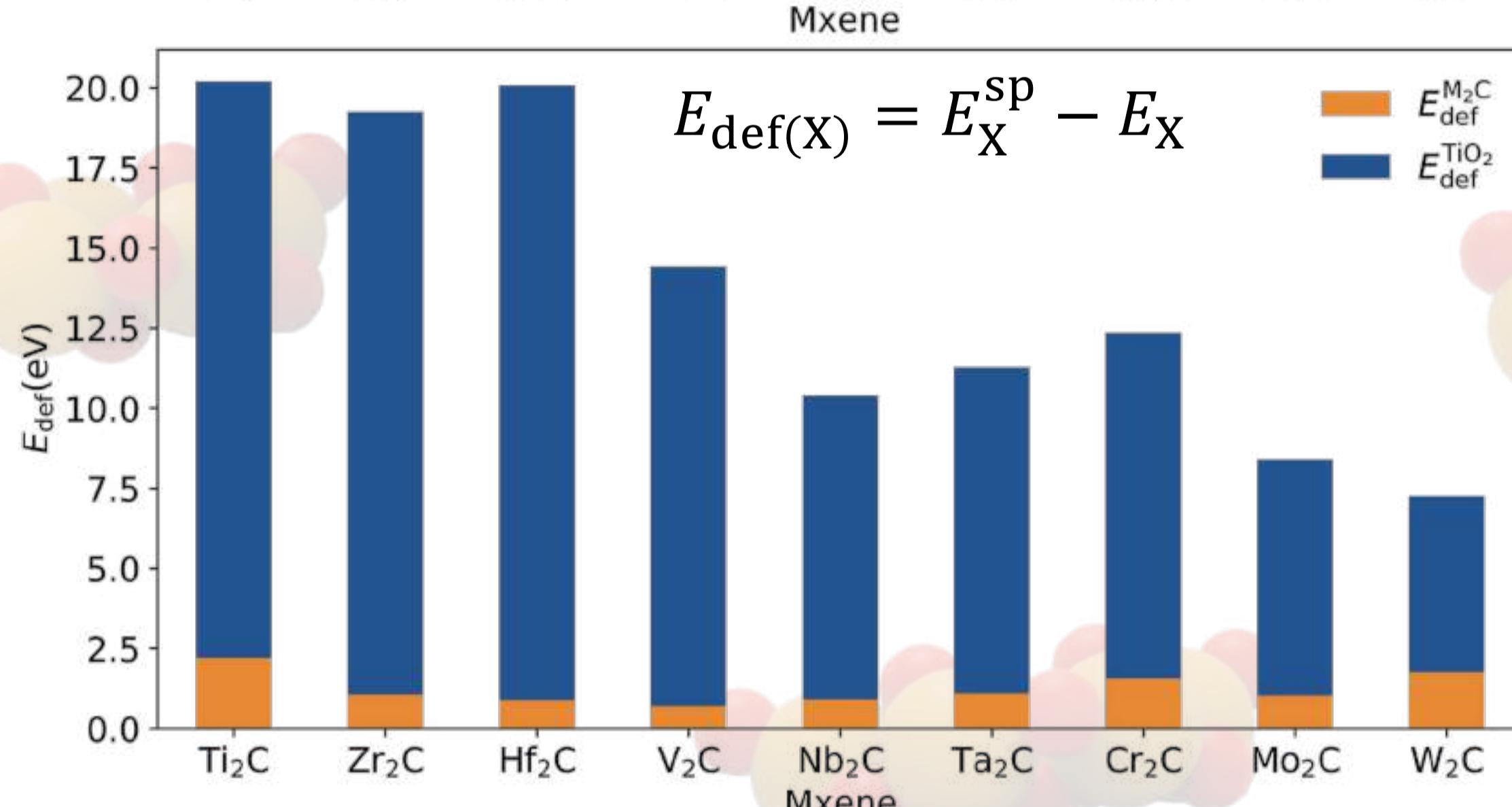
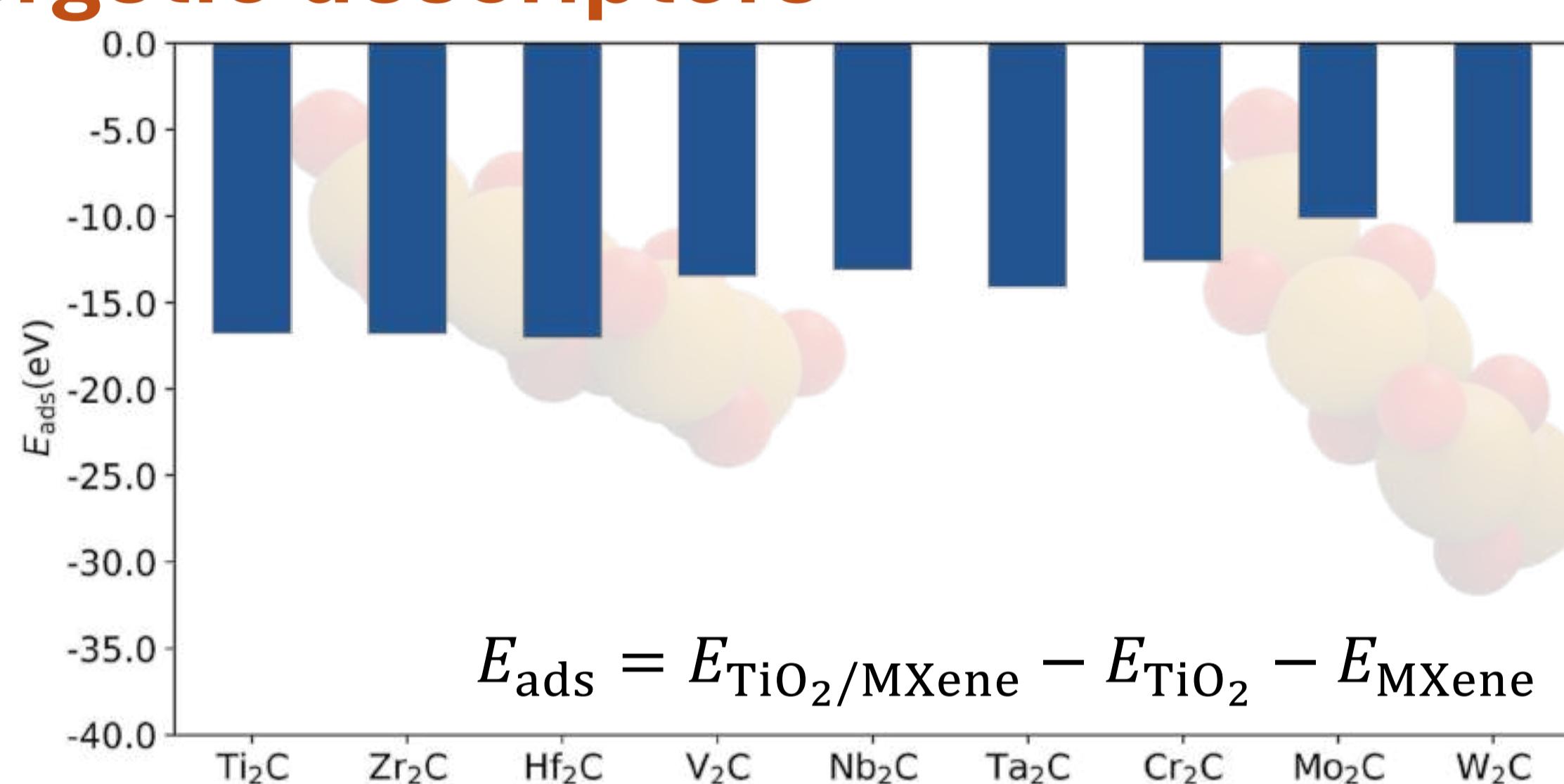
Motivation

TiO₂/MXenes heterostructures obtained *in situ* by **oxidation** of MXene surface.

Applications in photocatalysis: CO₂ reduction, H₂ generation, etc.[1,2]

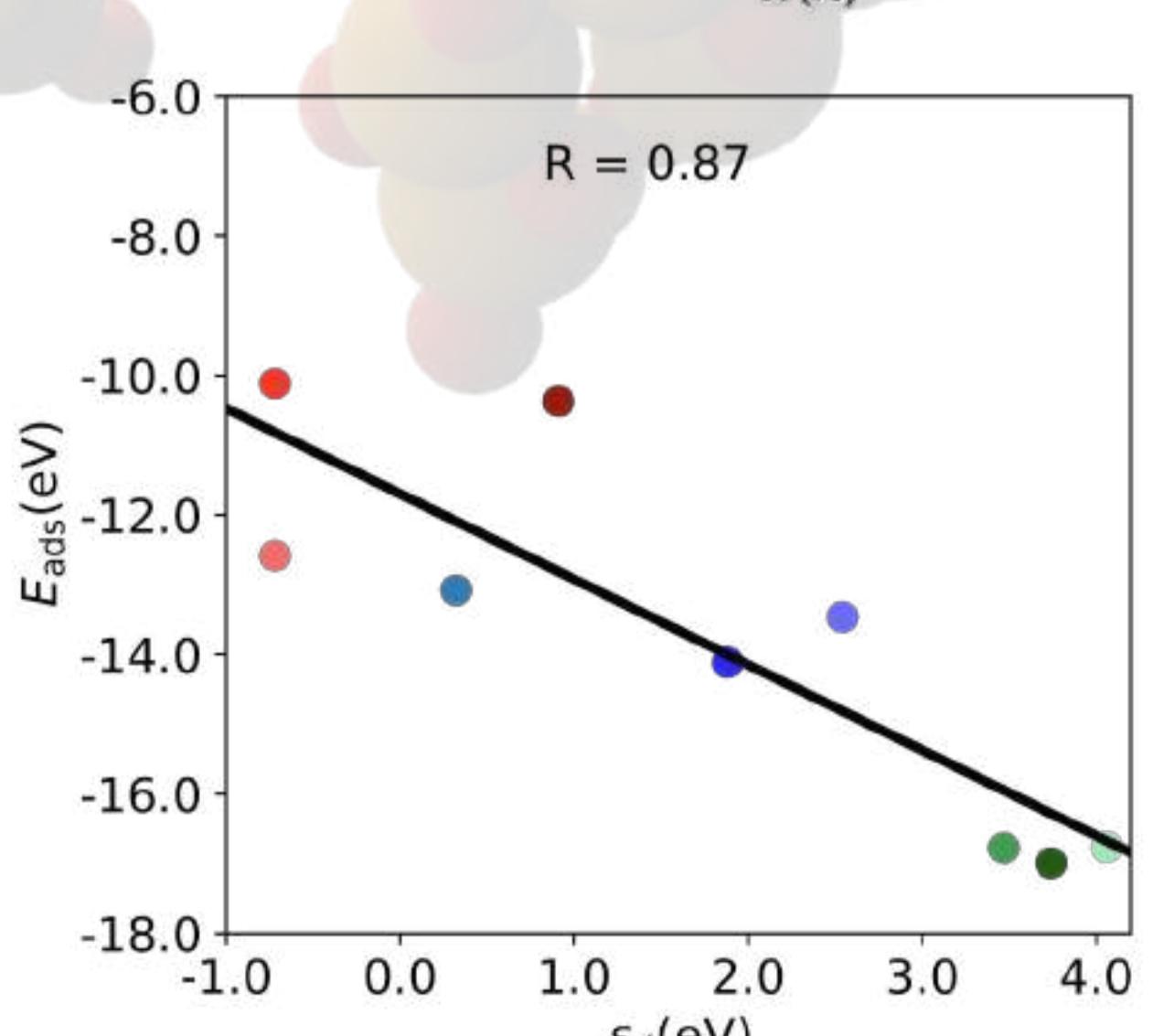
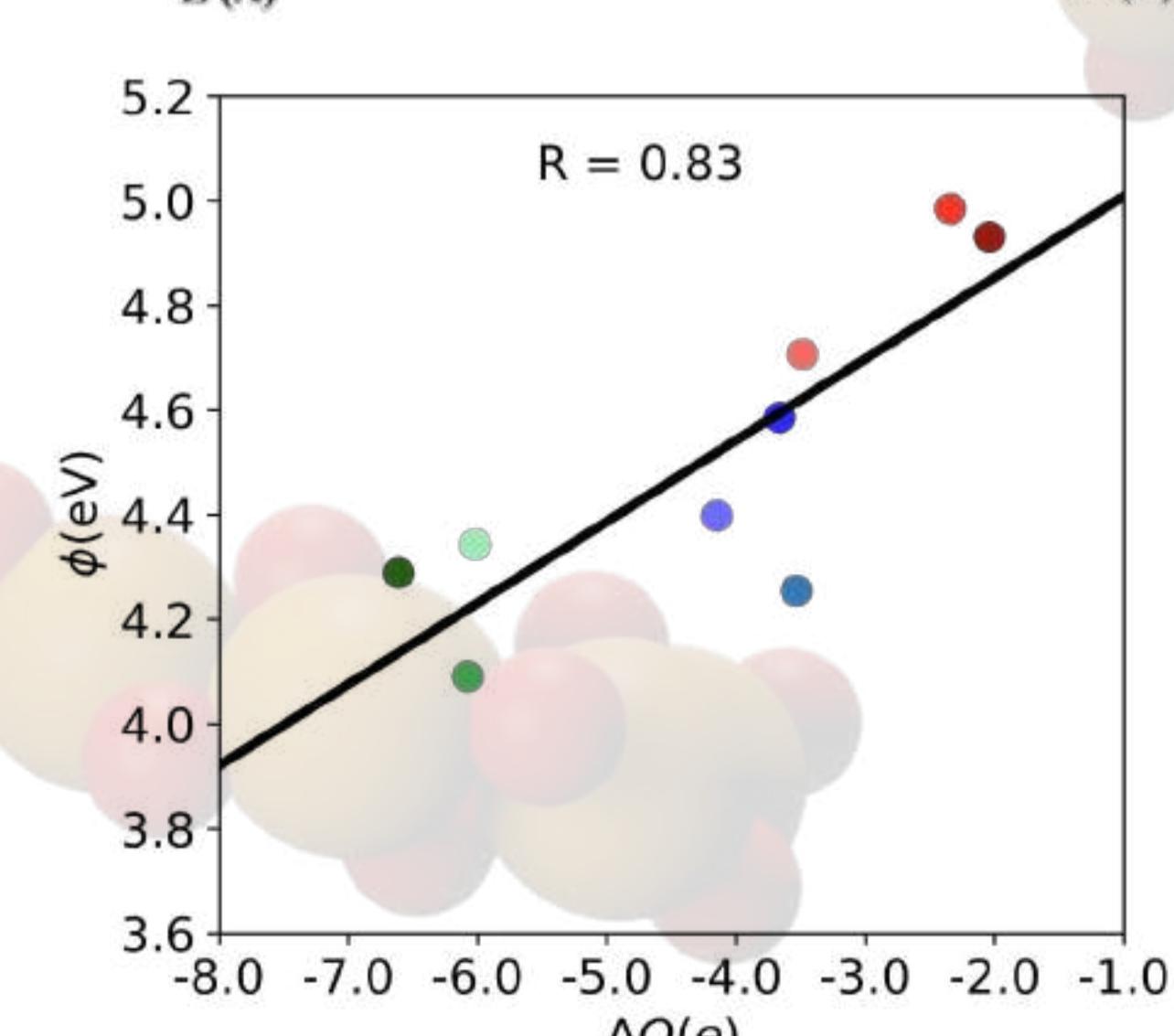
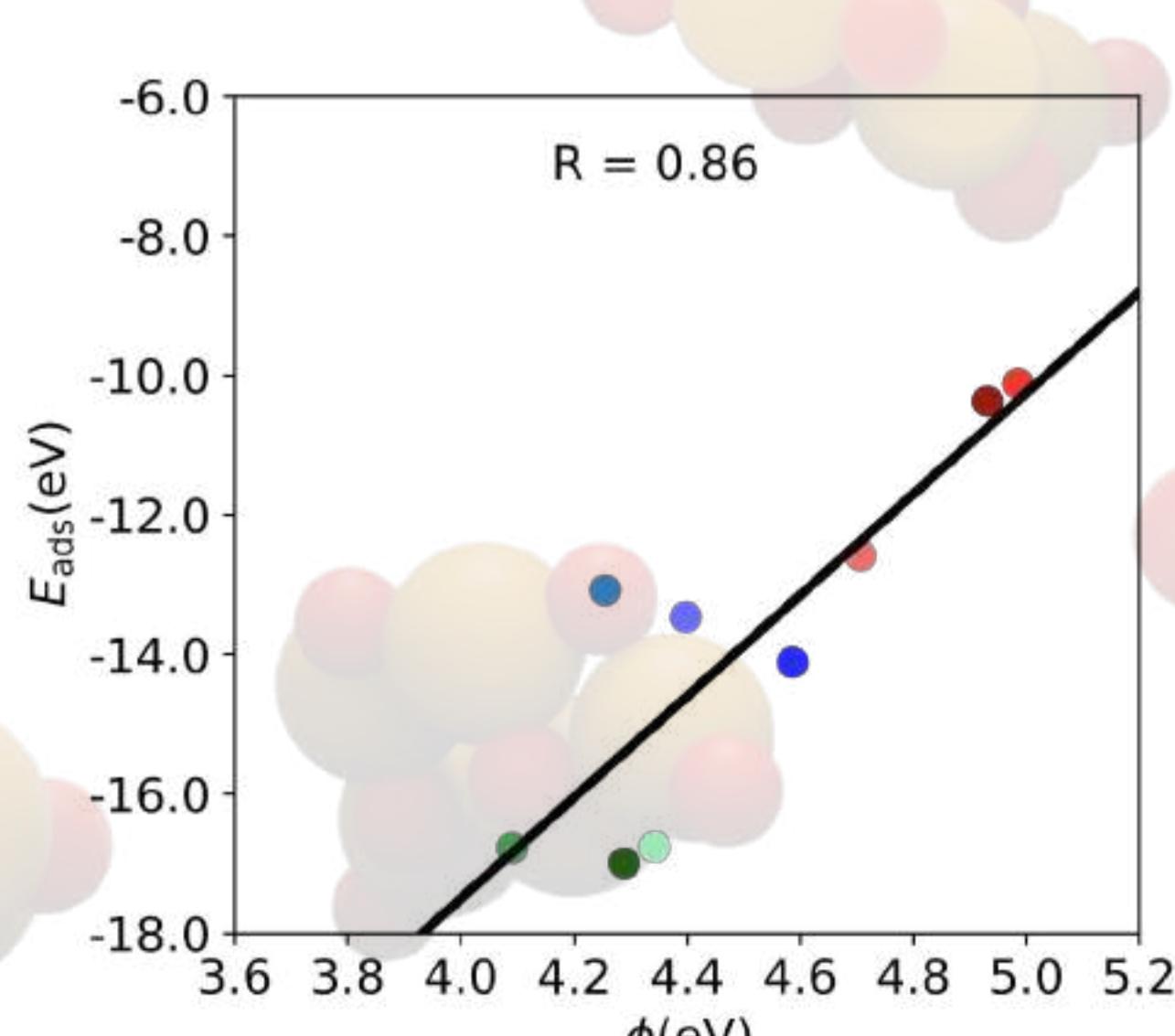
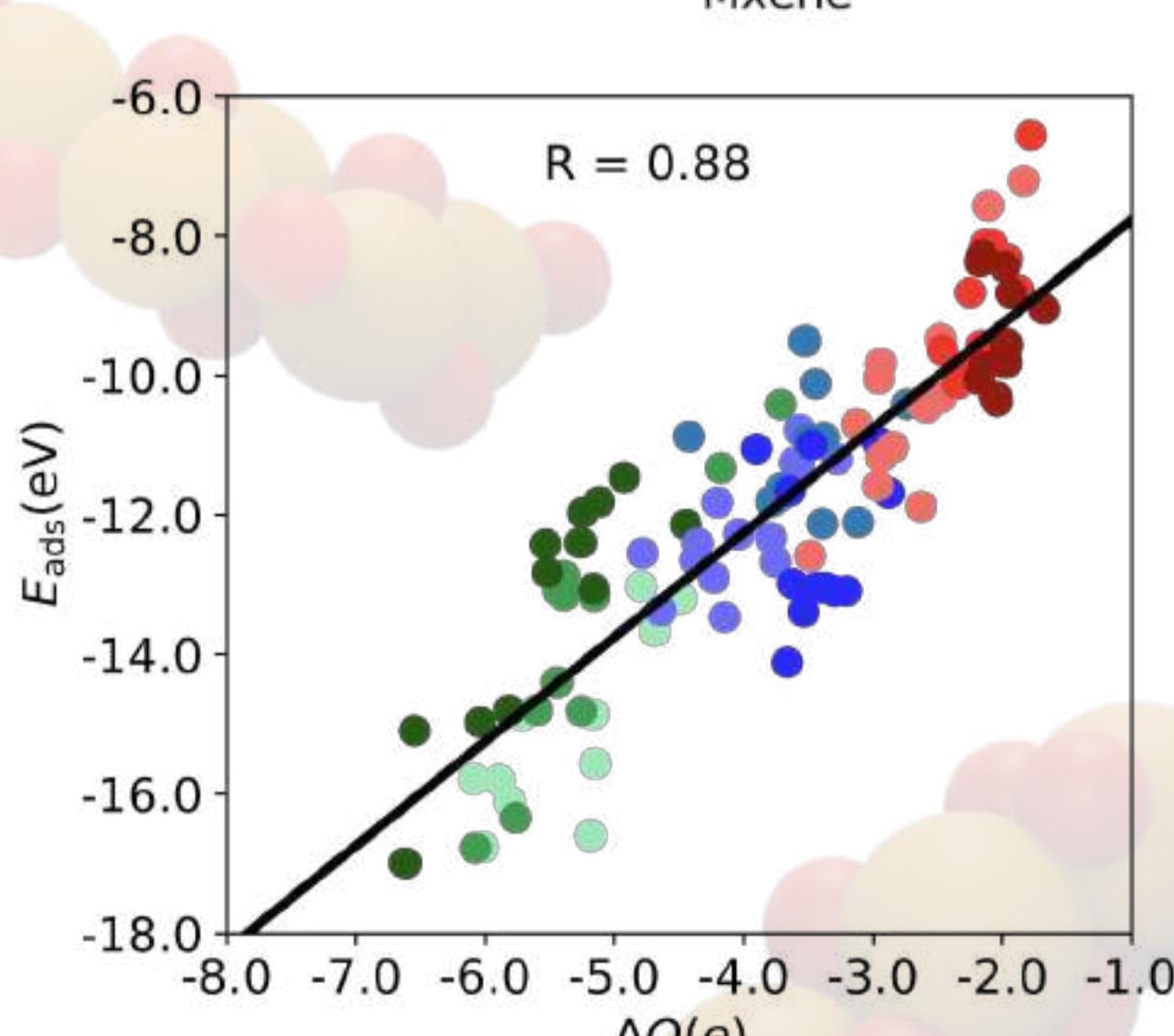
The effects of MXene metal composition on structural and electronic properties of TiO₂/MXene composites.

Energetic descriptors



Trends

- Ti₂C
- Zr₂C
- Hf₂C
- V₂C
- Nb₂C
- Ta₂C
- Cr₂C
- Mo₂C
- W₂C



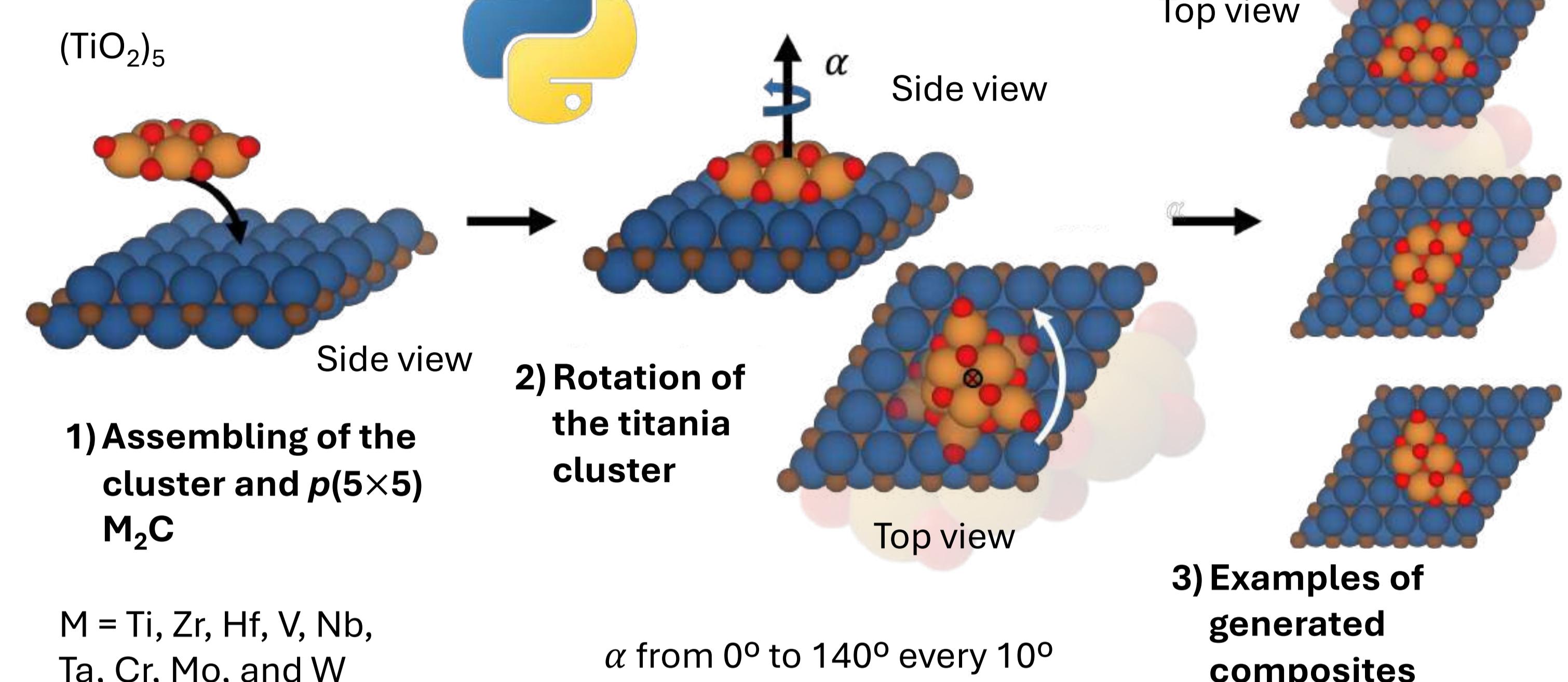
Conclusions

- Highly exothermic E_{ads} regardless MXene composition.
- $|E_{\text{ads}}|: d^3 > d^4 > d^5$.
- Charge transfer from MXene towards TiO₂ regardless MXene composition.
- Features of the metal element in the MXene can be employed to predict trends.[4]

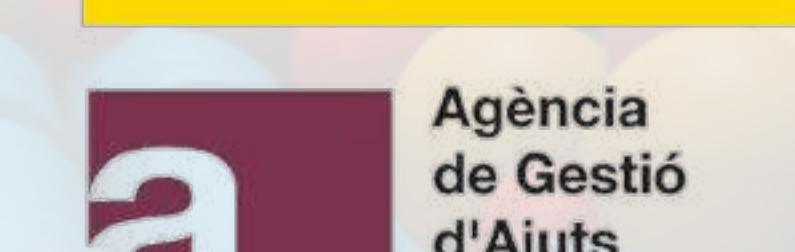
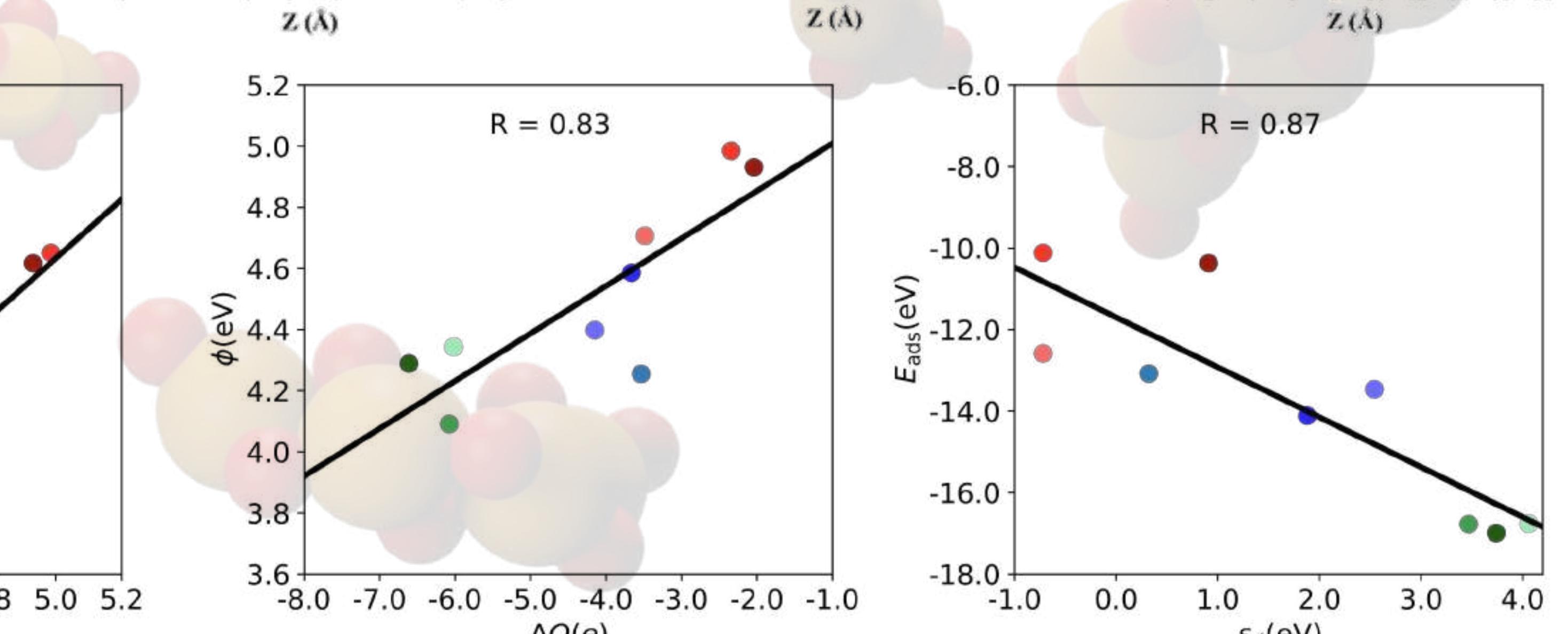
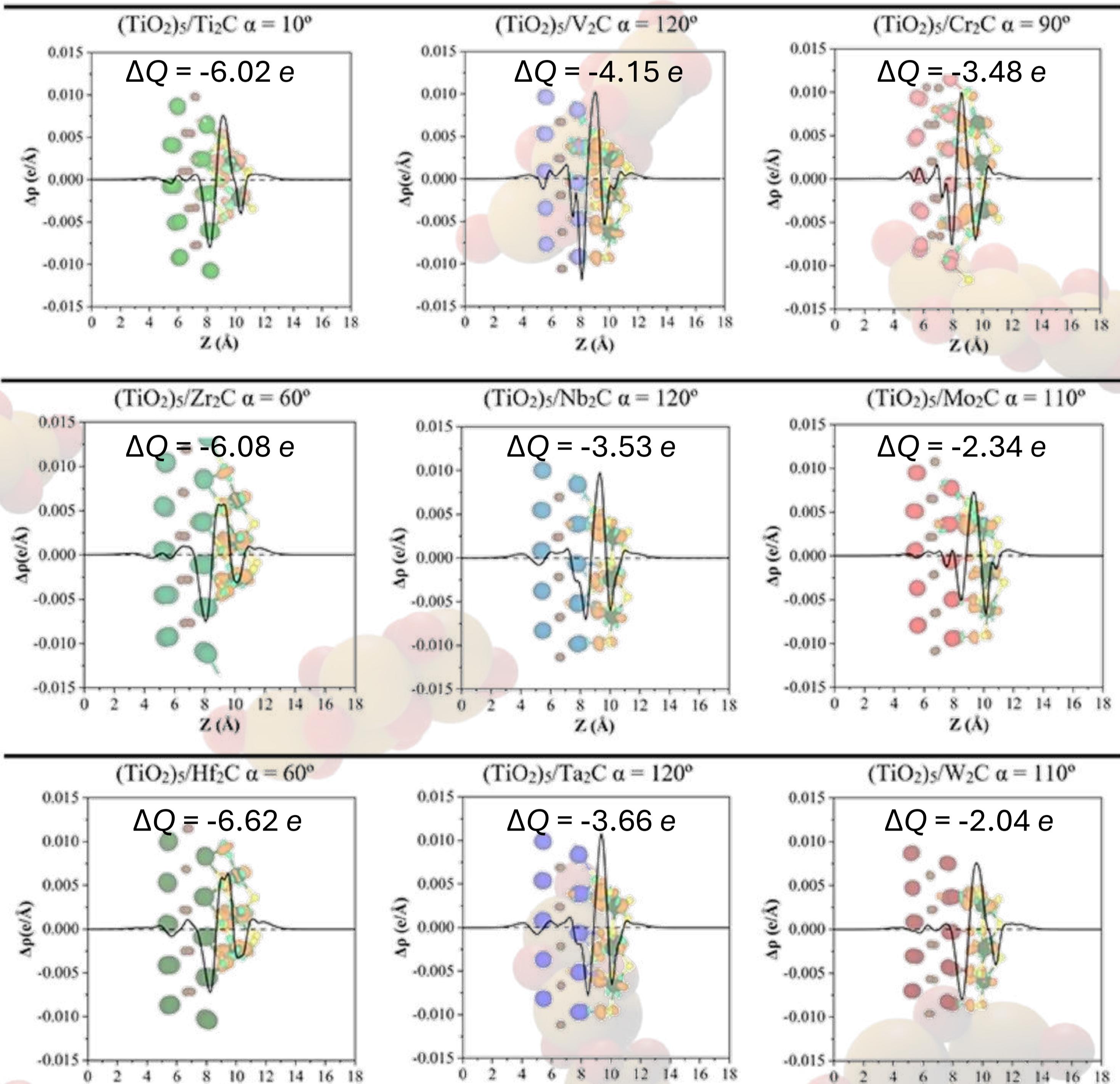
References

- [1] J. Low, et al. *J. Catal.*, **2018**, *361*, 255–266.
- [2] T. Su, et al. *ACS Appl. Energ. Mater.*, **2019**, *2*, 4640–4651.
- [3] N. García-Romeral, et al. *Chem. Eur. J.*, **2024**, *30*, e202400255.
- [4] M. Keyhanian, et al. *Phys. Chem. Chem. Phys.*, **2024**, *26*, 25319–25328.

Models [3]



Interface polarization



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