

Overview on Research

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Group



Nachtigall's group and CUCAM



Personal Background



Master and Bachelor in Milan Bicocca (IT), PhD in Bath (UK),
PostDoc experience (Cambridge (UK) and Prague (CZ)).

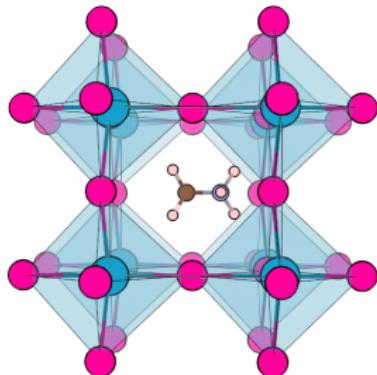


PhD topic



Hybrid perovskites- MAPI (MAPbI_3):

- ▶ Electronic structure
 - Standard DFT
 - SOC correction
 - Rashba Splitting
 - GW
- ▶ Vibrational properties
 - Different phase analysis
 - Dynamical behaviour
- ▶ Alloying
 - Quasi-chemical approximation
 - Role of impurities

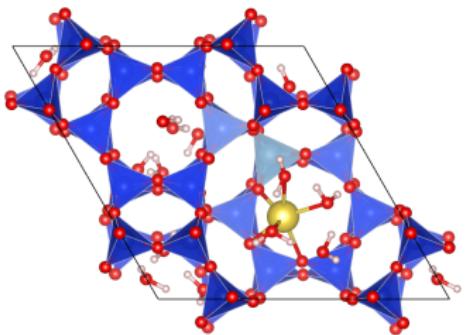


Zeolite NMR



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Focus on Catalysis: description/characterization of local environment.
Interpretation of MD and NMR.

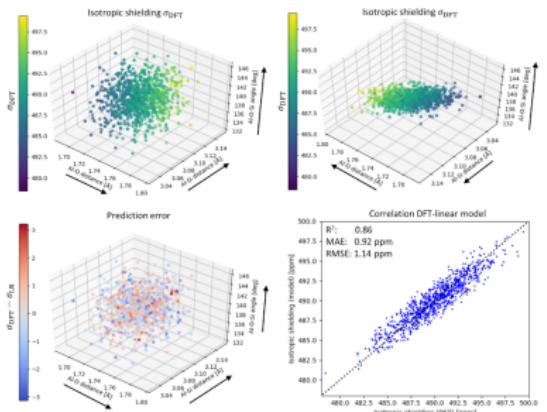


- ▶ Simulation of **realistic** NMR
(pH, water loading, counter cation, ...)
- ▶ ²⁷Al-NMR, resolution of quadrupolar-coupling
- ▶ NMR Tensors from t-average of *ab-initio* MD
- ▶ Several FrameWorks: CHA, MOR, MFI
- ▶ Experimental interpretation

Zeolite collaboration



NMR has several implications



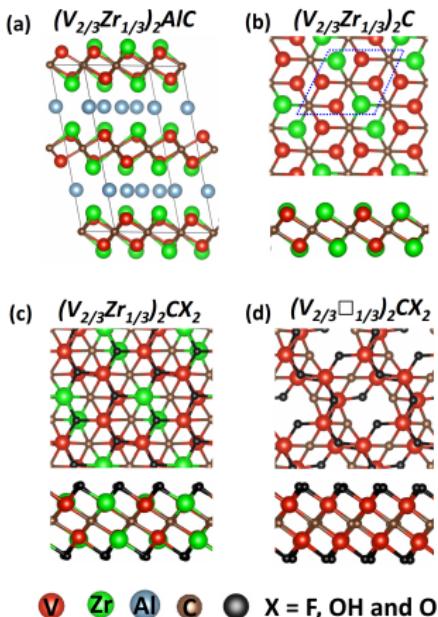
- ▶ Collaboration with experimental group in St. Andrews (SCO)
 - ▶ SIMPSON for full spectra analysis
 - ▶ Neural Network to build multidimensional prediction of NMR/EFG tensors
 - Mining past MD run
 - Extension to large-scale simulations
 - Improvement on past single parameters fitting

MXenes



Electronic and magnetic properties of MXenes

- 2D material related to MAXI phase
- Graphene-like structure
- Spintronic - valletronics
- Rich stoichiometry
 - a. alloying
 - b. systematic vacancies
 - c. surface functions



Results

Check of stability (vibrational spectra) and control of electronic properties with stoichiometry and surface functions.

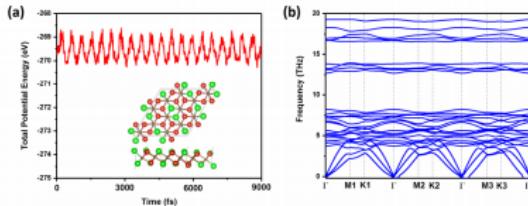
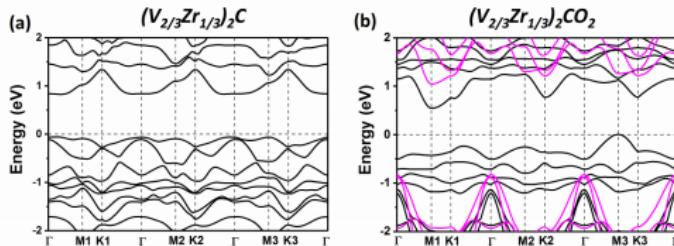


Figure S5: (a) Variations of the total potential energy of $(V_{2/3}Zr_{1/3})_2C$ during ab initio molecular dynamics simulations at 300 K. (b) Phonon dispersion curves for $(V_{2/3}Zr_{1/3})_2C$.

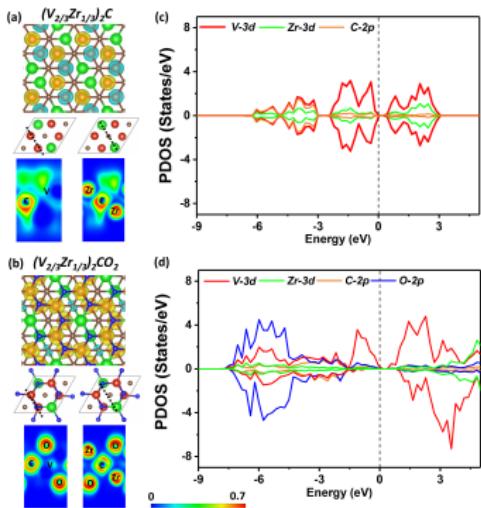
The inclusion of O functional breaks the AFM ordering



DOS



Example $(V_{2/3}Zr_{1/3})_2C$ vs $(V_{2/3}Zr_{1/3})_2CO_2$
Proper description obtained using DFT+U model and Hybrid functionals



- ▶ Pristine MXene is semiconductor with AFM character
- ▶ O_2 shift the d-levels -> FM
- ▶ O_2 half-semiconductor

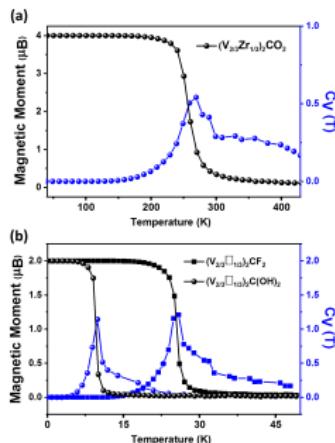
Ising Model



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Example $(V_{2/3}Zr_{1/3})_2C$ vs $(V_{2/3}Zr_{1/3})_2CO_2$

- O induce shift only in one spin channel, inducing a FM GS
- Mostly due to charge redistribution on the surface - affects the V atoms d levels
- Similar behaviour of depletion of d orbital and presence of vacancies
- AFM is usually the GS for others $(V_{2/3}Zr_{1/3})_2CX$

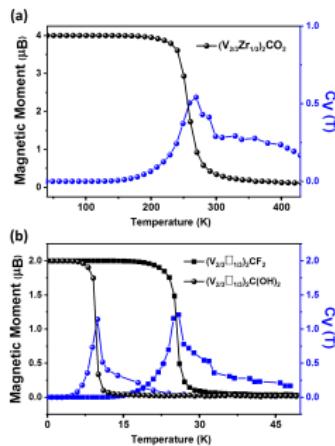


Surface function



Example $(V_{2/3}Zr_{1/3})_2C$ vs $(V_{2/3}Zr_{1/3})_2CO_2$

- From DFT, Monte Carlo can estimate Curie T
- Surface functionalization can control behaviour!
- The behaviour **NOT** trivial as second case show!
 - a. Surface effect (dipoles, field,...)
 - b. magnetic interaction
 - c. Charge distribution

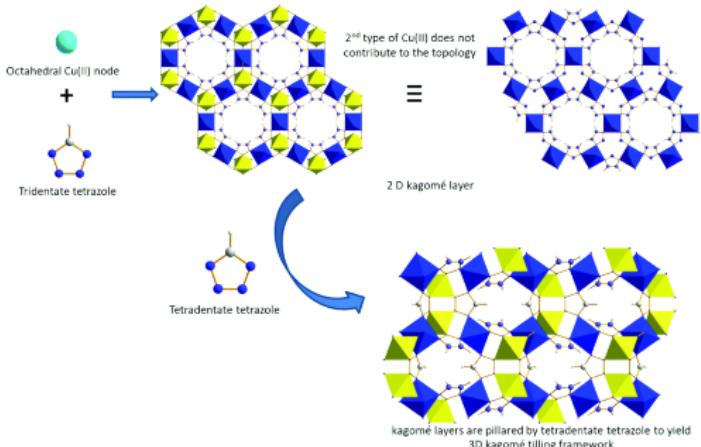


Kagome-MOF



We considered two **new synthetized MOF** with *Kagome* lattice with Cu and Co as metal center, linker: tetrazole-5-carboxylate ethyl ester

- ▶ Structure hexagonal lattice
- ▶ Very stable (Solvent, pH, T)
- ▶ **Magnetic properties**





Cococcioni's Method

Hubbard scheme has some limitations:

- ▶ Semi-empirical
- ▶ Constant correction

The idea: effective Hubbard parameter system dependent! Performed at a linear response regime

$$U_I = \frac{\partial E^{GGA}}{\partial(n^{If})^2} - \frac{\partial E_0^{GGA}}{\partial(n^{If})^2} = \chi_0^{-1} - \chi^{-1} \quad (1)$$

Specific for your system!

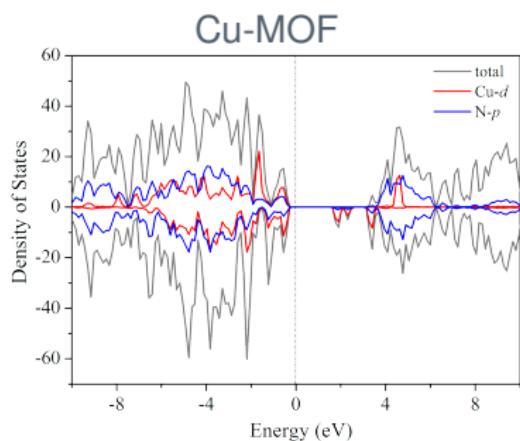
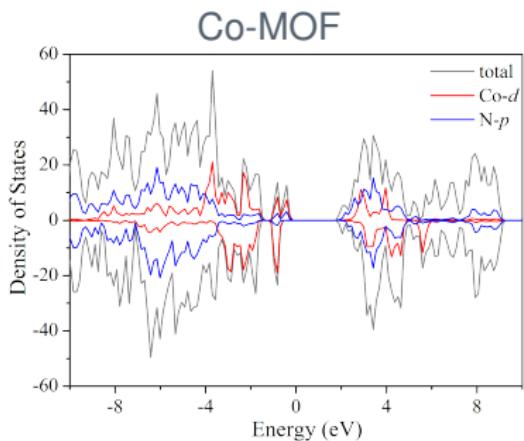
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Cococcioni's Method Results



1. Hybrid functional did not converge (\rightarrow we did not try to change HF-parameter)
2. GGA+ U_C also did not

We as a last resort used HSE06+U (Cococcioni)



Acknowledgment



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