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Tuning the electronic, magnetic and optical properties of 2D materials: *Ab initio* insights

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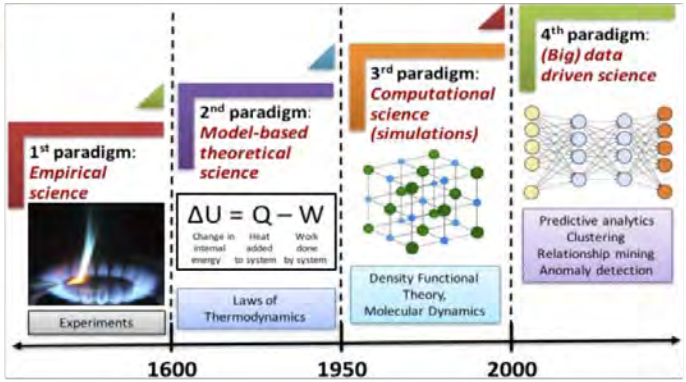
Introduction

There are several competing RESEARCH PARADIGMS when it comes to investigating properties of novel materials

The main drive behind these different paradigms is fuelled by the desire to design the *next generation* of materials/systems with *novel properties* needed for *novel applications* through;

- *Tuning* a material specific property to yield a desirable effect
- *Tuning* a material specific property to yield an effect observed another material but at lesser cost or improved efficiency

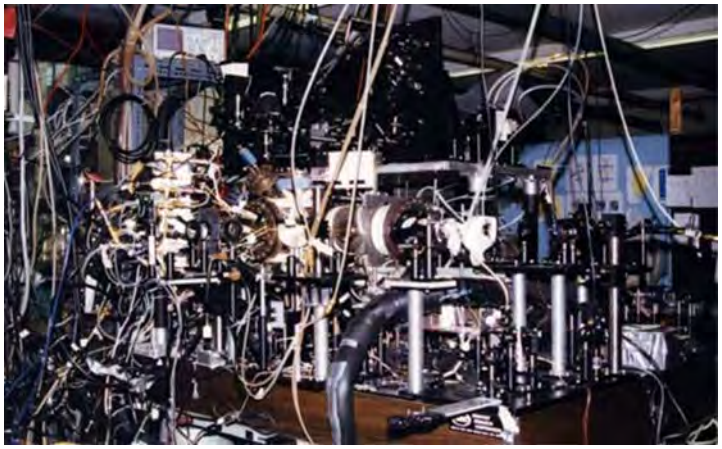


A. Agrawal, A. Choudhary, APL Mater. 4 (2016) 53208.
R. Seshadri, T.D. Sparks, APL Mater. 4 (2016) 53206.

Hypothesis testing

According to the experimentalist/empiricist …

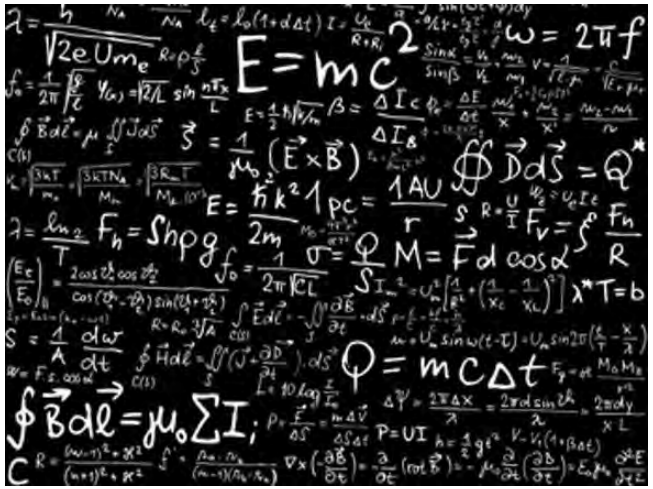
How is a hypothesis tested



Hypothesis testing …

According to the theorists …

How is a hypothesis tested



2nd paradigm:
Model-based theoretical science

Laws of Thermodynamics

Hypothesis testing …

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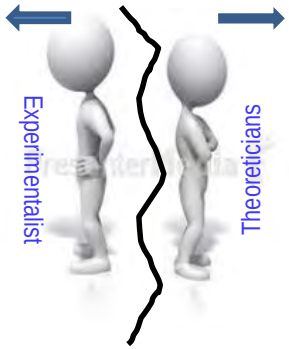
And then …

Experimental meetings



Theoretical meetings

Competing interests!!!

NOT ALL EXPERIMENTALLY OBSERVED PROPERTIES CAN BE MODELLED AND ALSO NOT ALL MODELLED PROPERTIES CAN BE MEASURED EXPERIMENTALLY

Hypothesis testing …

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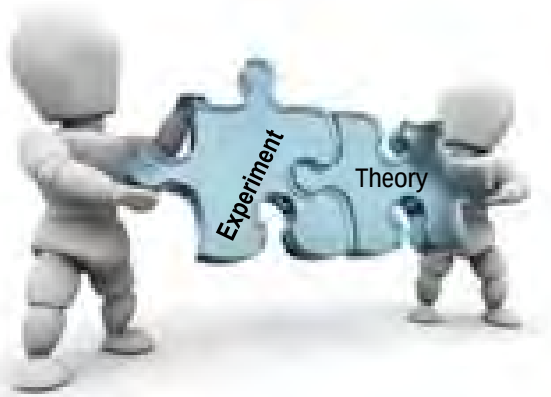
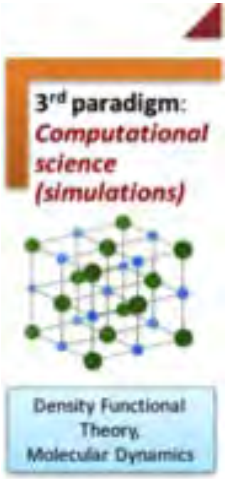
The birth of computational modelling



Supercomputing

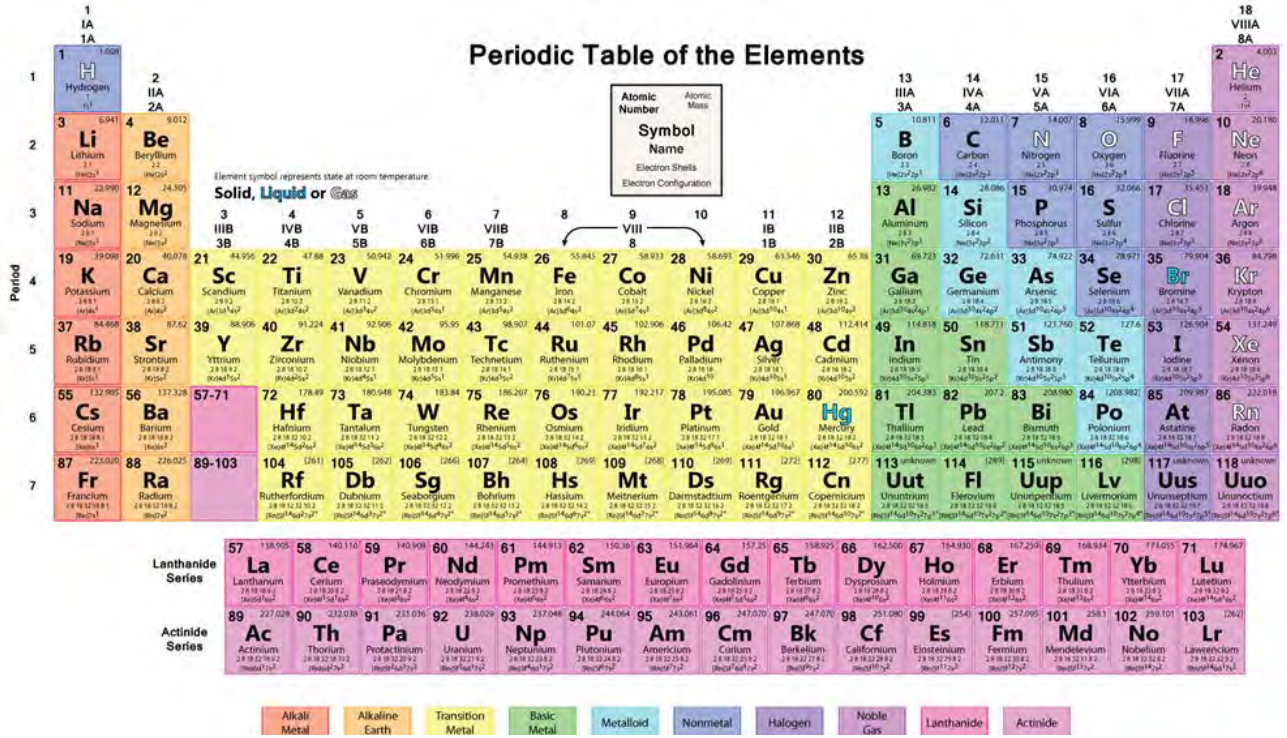


Objective was to;

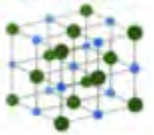
- carry out complementary investigations (theory + experiments)
- test developed theories (*limits and boundaries/Applicability domains*)
- provide fundamental explanations to experimentally observed phenomena
- design novel experiments

Why computational …

Too many elements to be considered …



3rd paradigm: *Computational science (simulations)*

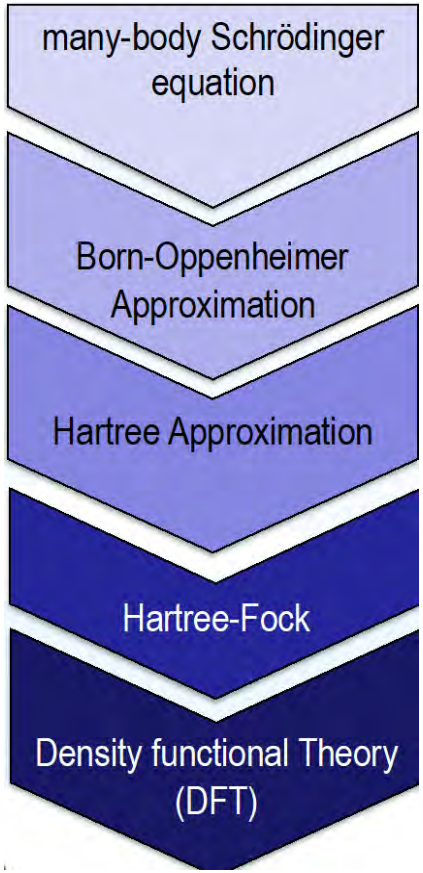


Density Functional Theory, Molecular Dynamics

- *Intrinsic* material *properties* are governed by the *intrinsic characteristics* of the elements forming the material
- Doping has been *successful* to some extent in *improving* the materials' properties
- NOT all materials can be supper materials

Computational methodology…

- *Ab initio* formalism

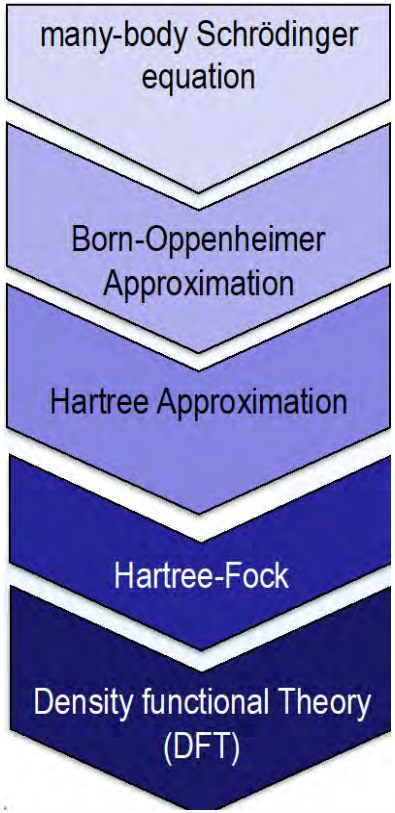


- If the ground-state charge density of a system is known, all the properties of the system can be determined
- The energy associated with the ground state of system is the ground-state energy

This is just one approach for computational modelling others do exist

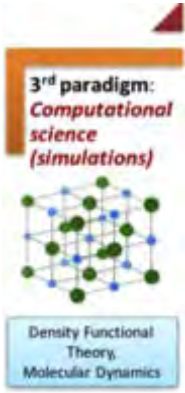
Computational methodology…

- *Ab initio* formalism



- If the ground-state charge density of a system is known, *almost* all the properties of the system can be determined

Need to go beyond DFT



This study ...

Application of ab initio DFT modelling to

1. Defects in 2D materials (semiconductors)
   - Transition metal dichalcogenides (TMDC): MoS2,TcS2, ReX2
   - Graphene and Holey doped graphene
   - g-III-IV compounds (AlN, GaN and InN)
2. van der Waals heterostructures

Computational packages/CODES used

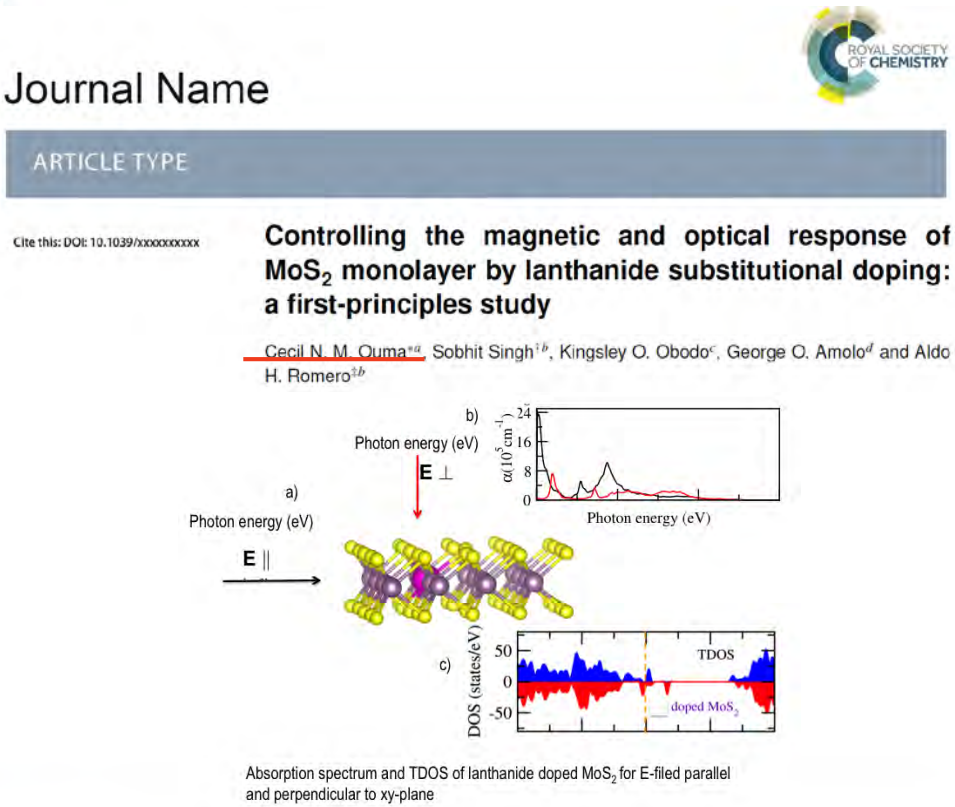
Quantum ESPRESSO (PWSCF)

Properties investigated

1. Formation energies
2. Optical properties
3. *Binding energies*
4. *Migration energies*

Applications

CASE 1: (Collaborative project on lanthanide doped TMDCs (MoS2))



Absorption spectrum and TDOS of lanthanide doped MoS_2 for E-filed parallel and perpendicular to xy-plane

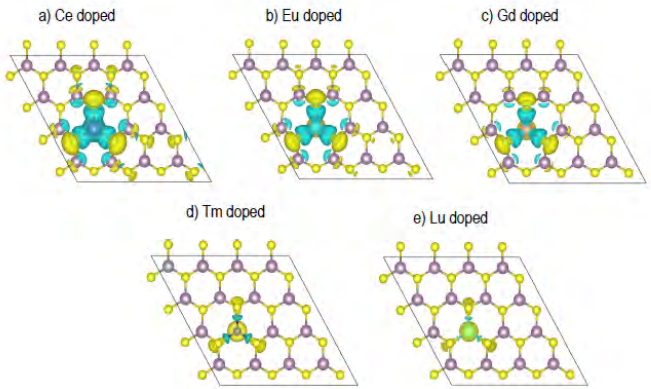
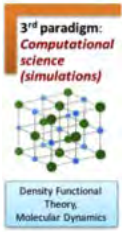


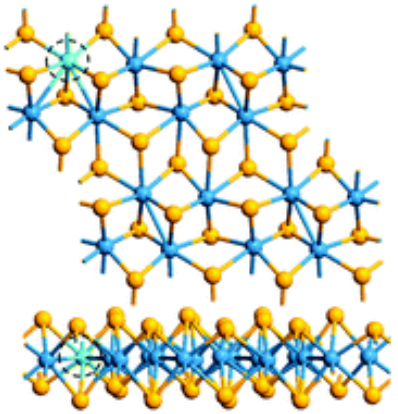
Fig. 3 Charge density difference plots for a) Ce-doped, b) Eu-doped, c) Gd-doped, d)Tm-doped, and e) Lu-doped MoS2 monolayer.

Lanthanide dopants
Ce, Eu, Gd, Tm and Lu



Applications

CASE 1: (Collaborative project on transition metal doped TMDCs (ReS2 and ReSe2))



PCCP

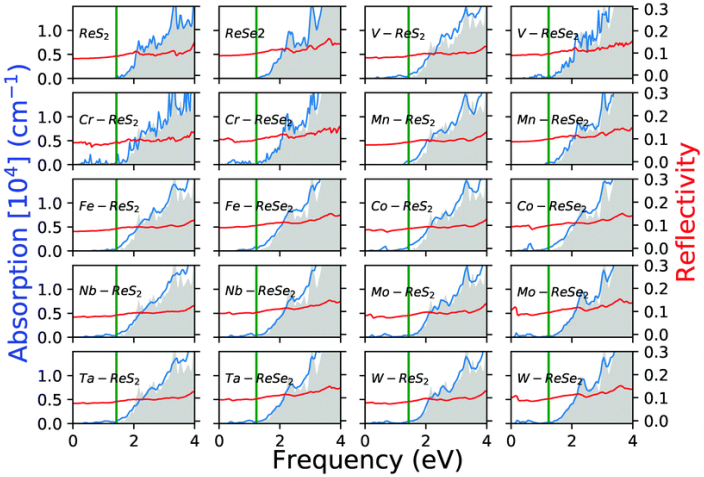
PAPER

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2017, 19, 19050

Influence of transition metal doping on the electronic and optical properties of ReS_2 and $ReSe_2$ monolayers

Kingsley Onyebuchi Obodo, *[a] Cecil Napthaly Moro Ouma,[b] Joshua Tobechukwu Obodo[c] and Moritz Braun[d]



Transition metal dopants
V, Cr, Fe, Nb, Ta, Mo and W

3rd paradigm: *Computational science (simulations)*

Density Functional Theory, Molecular Dynamics

Applications

CASE 3: (Collaborative project on transition metal dopants and adatoms TMDCs (TcS2))

Journal Name

ROYAL SOCIETY OF CHEMISTRY

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Effect of transition metal substitutional dopants and adatoms on mono layer TcS_2: *ab initio* insights †

Cecil N. M. Ouma,*[a], Kingsley O. Obodo[b], Sobhit Singh[c], Moritz Braun[b] and George O. Amolo[d]

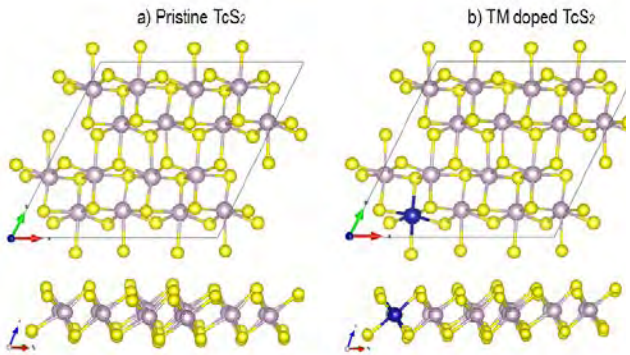


Fig. 1 Top and side view of the optimized crystal structures of pristine and transition metal (TM) doped TcS_2. (Blue ball represents the substitutional dopant on a Tc site)

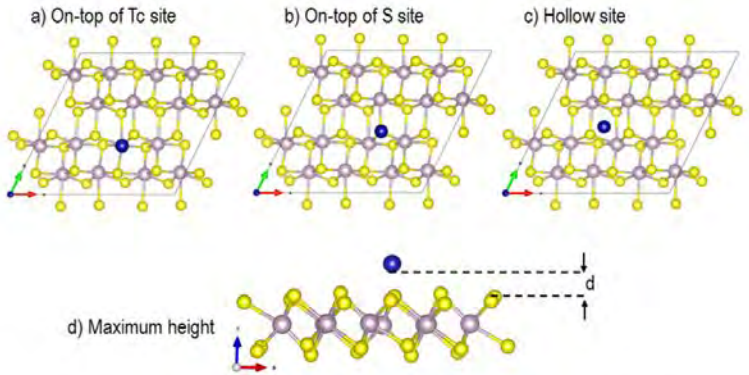


Fig. 2 Transion metal adsoption site considered namley on-top of Tc, (T_{Tc}) on-top of S (T_S) and the hollow position (H) (Blue ball represents the adatom and d is the distance between the adatom and the TcS_2 surface)

3rd paradigm: *Computational science (simulations)*

Density Functional Theory, Molecular Dynamics

Applications

CASE 4: (Collaborative project on graphene like AlN (g-AlN))

In progress

Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Graphene/g-AlN van der Waals nanocomposite for rechargeable Li ion battery (LIB) anode: *Ab initio* insights†

Cecil N. M. Ouma,*a

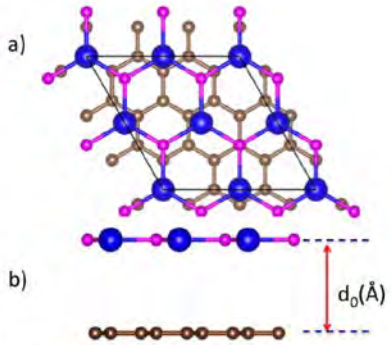


Fig. 1 Gr/g-AlN van der Waals nanocomposite. Blue, magenta and brown balls represents Al, N and C atoms respectively.

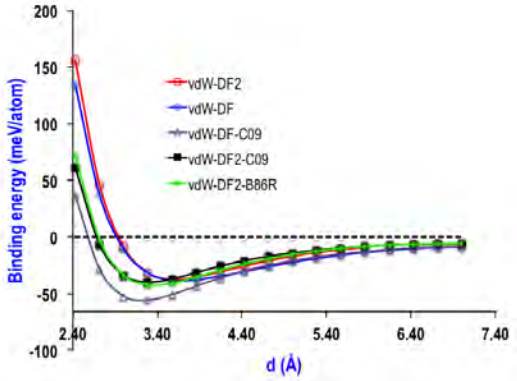
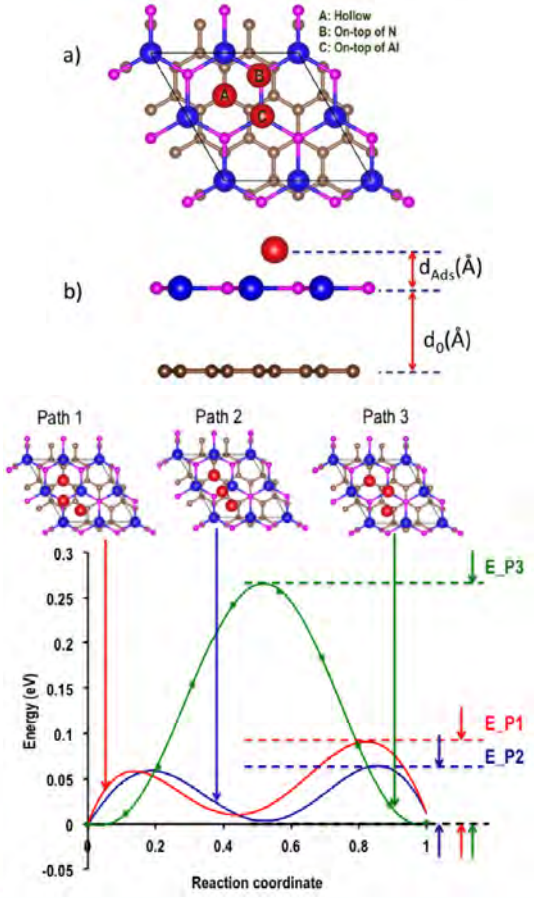
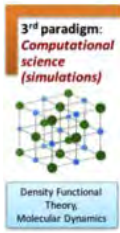


Fig. 2 Calculated binding energy if the Gr/g-AlN van der Waals nanocomposite as function of interlayer distance d for different vdW-D.





Applications

CASE 5: (Collaborative project on lanthanide embedded holey doped grapheme (g-C2N))

In progress

Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Tunable electronic and magnetic properties of mono-layer g-C_2N through embedding of lanthanide ions †

Cecil N. M. Ouma,*[a] and George O. Amolo[d]

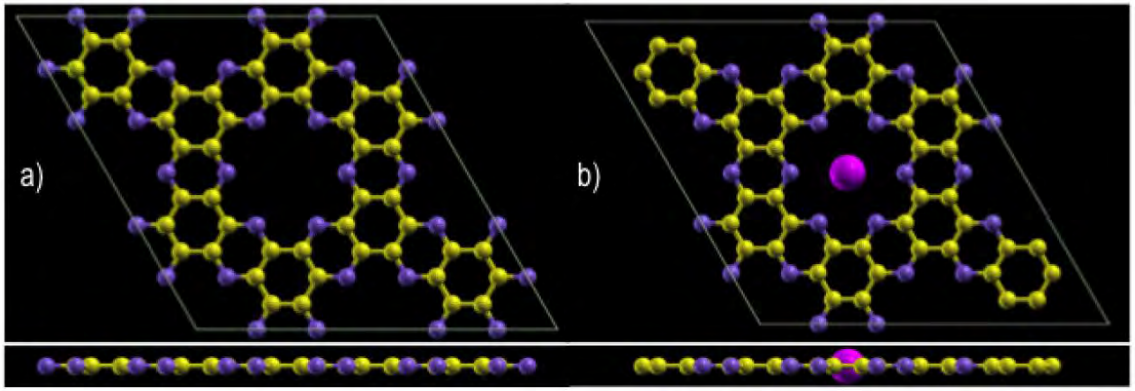


Fig. 1 : Top and side views of pristine and lanthanide emended g-C_2N. Gold, violet and magenta balls represents carbon, nitrogen and lanthanide atoms respectively.

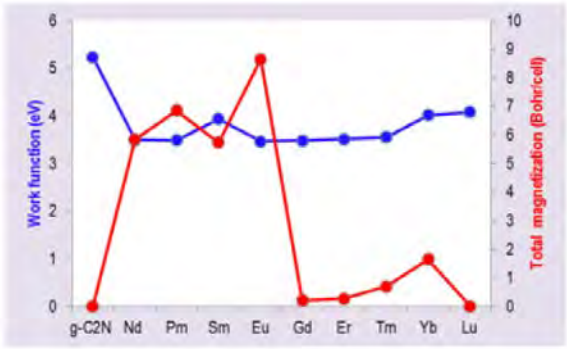


Fig. 6 Induced magnetization and calculated work function of lanthanide embedded g-C_2N.

3rd paradigm: *Computational science (simulations)*

Density Functional Theory, Molecular Dynamics

Conclusions

- Both lanthanide and TM doping influenced the optical properties 2D materials
- Both lanthanide and TM doping induced magnetism in 2D materials in some instances
- Its possible to create van der Waals heterostructures of of graphene and winde band gap monolayers of g-AlN
- Its possible to embed lanthanide ions in g-C2N

Ahsanteni sana …

Thank you for 

Any