ARTIFICIAL INTELLIGENCE IN HYBRID FUNCTIONALS FOR EXCITONIC PROPERTIES OF LOW-DIMENSIONAL SYSTEMS

MARENOSTRUM5 GPP

Led by



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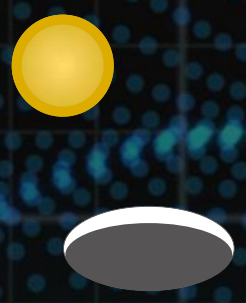
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1 WHAT ARE EXCITONS?



When **a photon excites an electron** in the valence band it leaves behind **a positively charged "hole"**

The electron and the hole can form **a bound state through Coulomb interaction**, which is called "exciton"

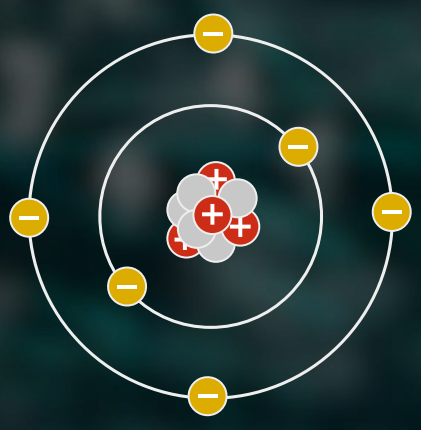


Excitons **can carry energy through a material without an electric current**, and improve the efficiency of devices such as solar cells

Understanding **how excitons form and break** holds huge potential for engineering the next generation of energy technologies



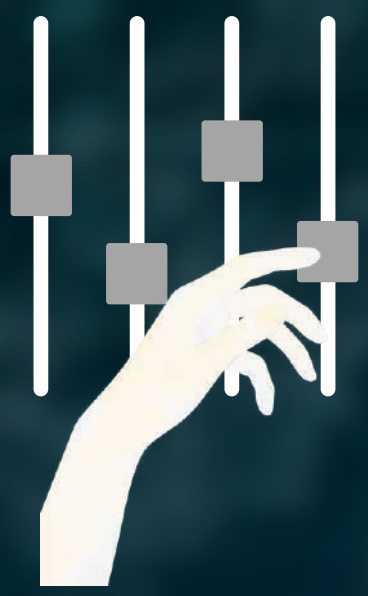
THE CHALLENGE OF STUDYING EXCITONS 2



Studying excitons requires to **calculate how electrons are arranged and their behaviour:** the electronic structure

Traditional methods are extremely computationally costly and are **very limited for large-scale studies**





One alternative is to combine hybrid functionals with time-dependent DFT, but it has one limitation: **they require material-specific parameters that require manual tunning**

3 TUNING EFFICIENTLY WITH AI METHODS

This project uses AI methods to **calculate these parameters automatically** without manual tuning





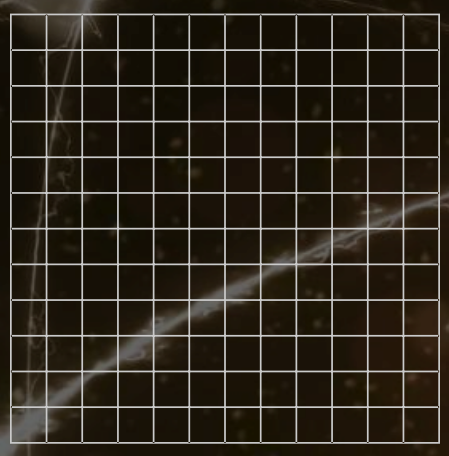
AI methods can find these parameters **maintaining the accuracy of theoretical calculations (ab initio)** with lower computational cost

MareNostrum5 was essential to calculate the traditional counterpart **for checking the method's validity**



CAN AI METHODS FIND THE CORRECT PARAMETERS?

4



The models successfully captured **the electronic structure of 2D materials** with ab initio accuracy

The approach **identified the correct parameters and calculated accurate electronic structures** necessary to determine excitonic properties





These AI methods are now integrated into the **‘EvoQuantum’ open software package** available for the scientific community

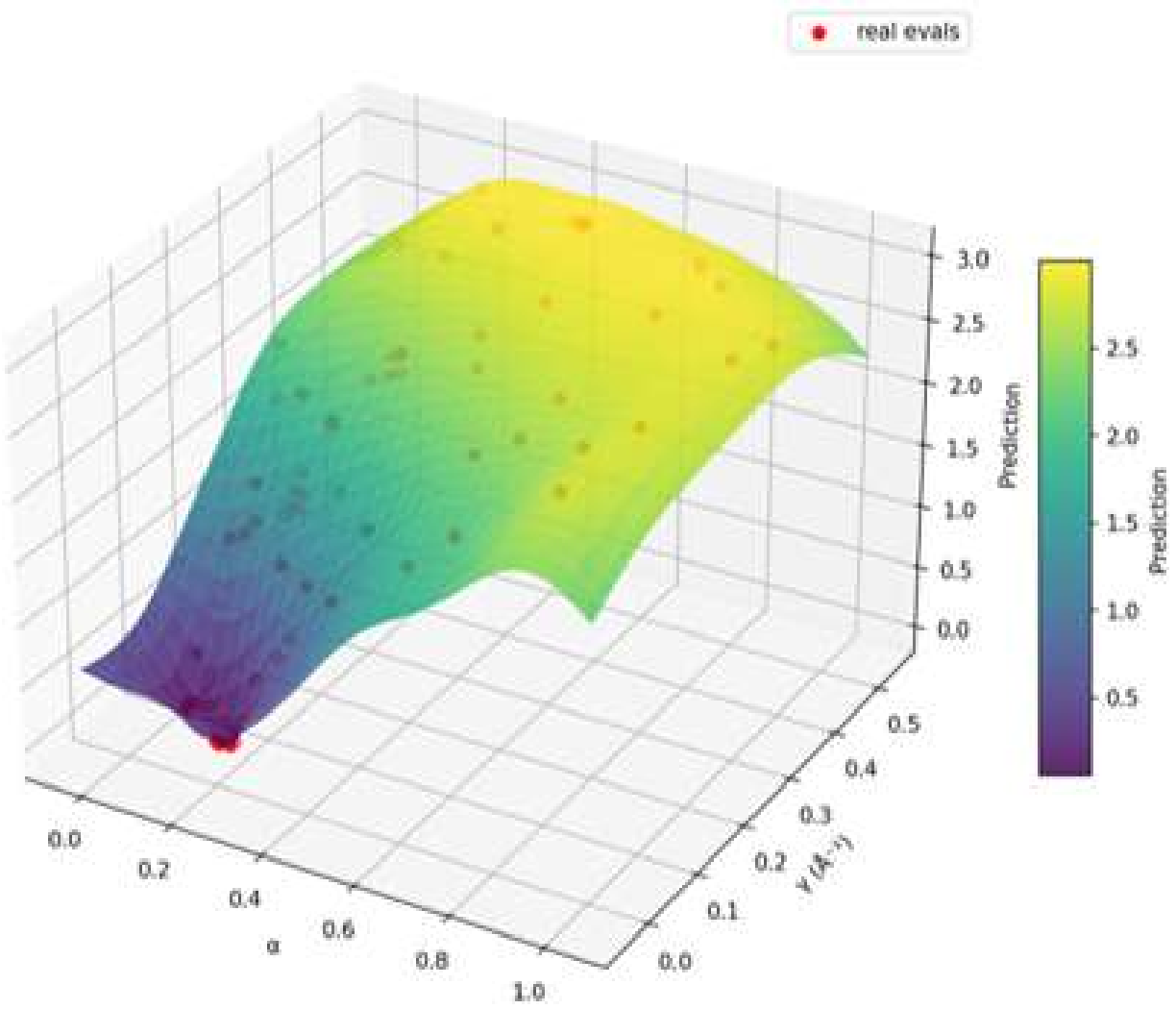


Figure. Energy landscape generated by a Gaussian Process (GP) surrogate model to determine the parameters (a, g) characterizing the band gap of a MoS_2 monolayer (calculated using a hybrid functional). **The red points** represent the real evaluations (real evals) obtained via Pattern Search, which served as the training data for the surrogate.

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