University of Antwerp

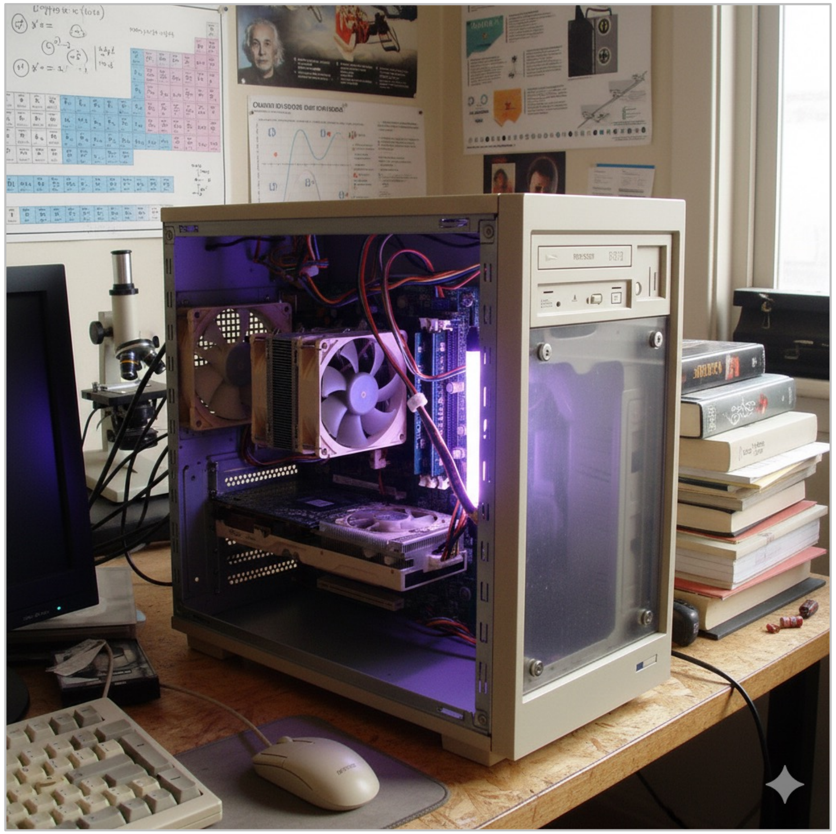
Computational Materials Modeling
for nanoscience and innovative technologies

Quantum Simulations and Machine Learning for Future Materials Technologies

Cem Sevik
Computational Materials Modelling Lab, Department of Physics,
University of Antwerp

Materials Modelling

2003 - High field transport phenomena in wide bandgap semiconductors.



Pentium 4 – 2GHz
512 MB RAM
Red Hat Linux

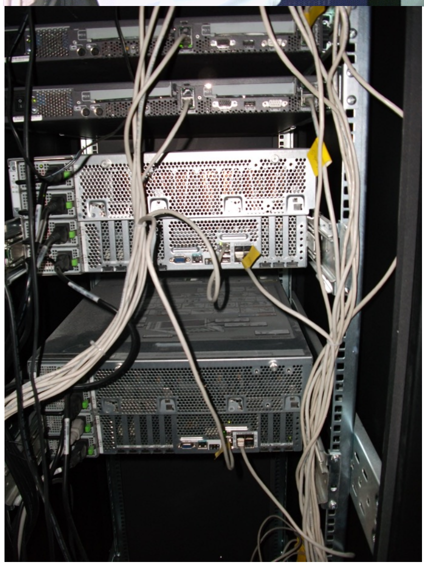
Materials Modelling

2008 -Carrier dynamics in silicon and germanium nanocrystals.

Pentium 4 – 3.4 GHz
1 GB RAM
GB Ethernet Connected
Red Hat Linux

Materials Modelling

2008 -Carrier dynamics in silicon and germanium nanocrystals.



5 Nodes

AMD Opteron 2 x dual-core

1 Node

AMD Opteron 4 x dual-core

8 GB

GB Ethernet Connected

Fedora

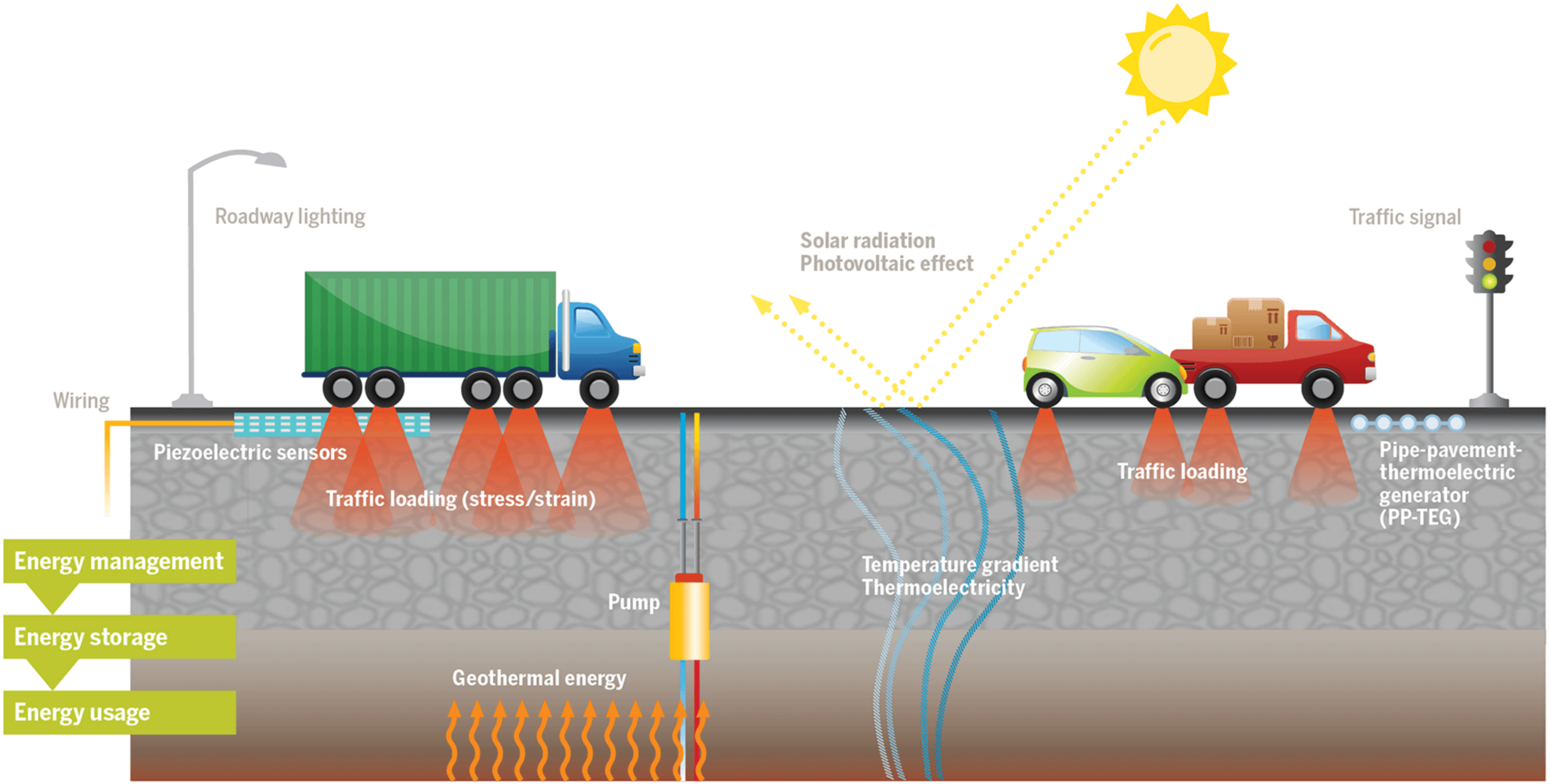
Materials Modelling

2012 – Electronic and thermal transport properties of 2D materials

15 Nodes
2 Intel Xenon E5 8 cores
64 GB
InfiniBand connected
Rock Cluster

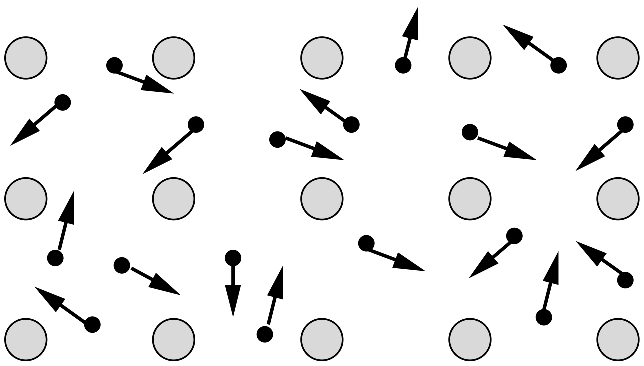
Materials Modelling

Why we need HPC power



https://cait.rutgers.edu/generating-power-every-time-you-hit-the-road/

Why we need HPC power



$$\widehat{H} = \widehat{H}_{\mathrm{e}} + \widehat{H}_{\mathrm{n}} + \widehat{H}_{\mathrm{n-e}}$$

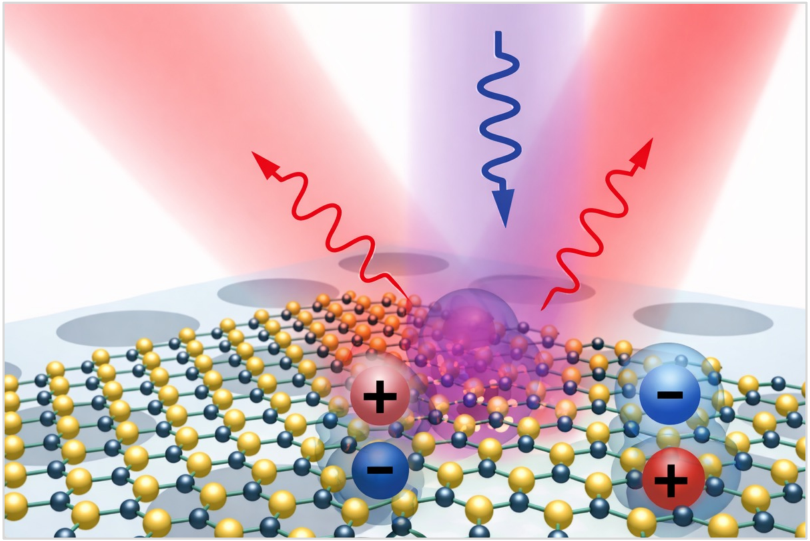
$$\widehat{H}_{\mathrm{e}} = \sum_{i} \frac{\widehat{\boldsymbol{p}}_i^2}{2m} + \frac{1}{2} \sum_{i \neq i'} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_{i'}|},$$

$$\widehat{H}_{\mathrm{n}} = \sum_{j} \frac{\widehat{\boldsymbol{P}}_j^2}{2M_j} + \frac{1}{2} \sum_{j \neq j'} \frac{Z_j Z_{j'} e^2}{|\boldsymbol{R}_j - \boldsymbol{R}_{j'}|},$$

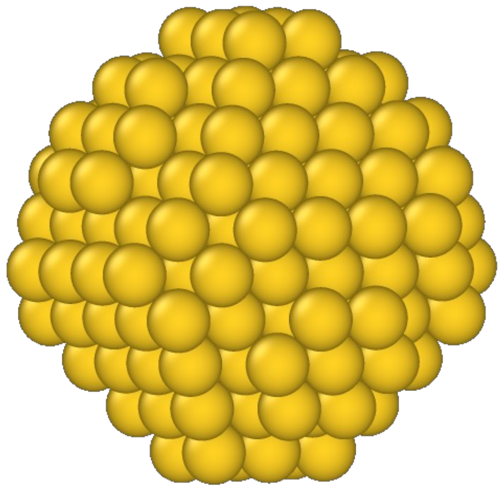
$$\widehat{H}_{\mathrm{n-e}} = -\sum_{i,j} \frac{Z_j e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_j|},$$

Why we need HPC power

Many – Body Quantum Simulations for Excitons



Machine Learning Interatomic Potentials for Materials



VLAAMS SUPERCOMPUTER CENTRUM

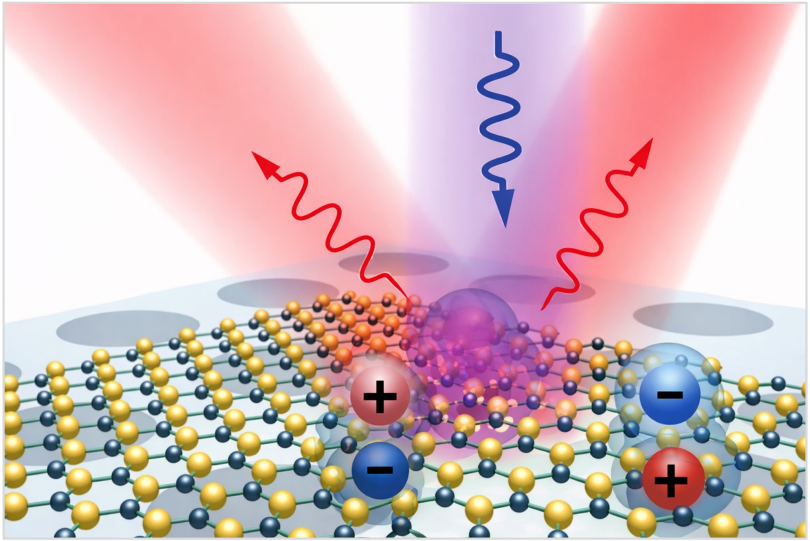
Vlaanderen is supercomputing

LEONARDO CINECA

LUMI

Why we need HPC power

Many – Body Quantum Simulations for Excitons



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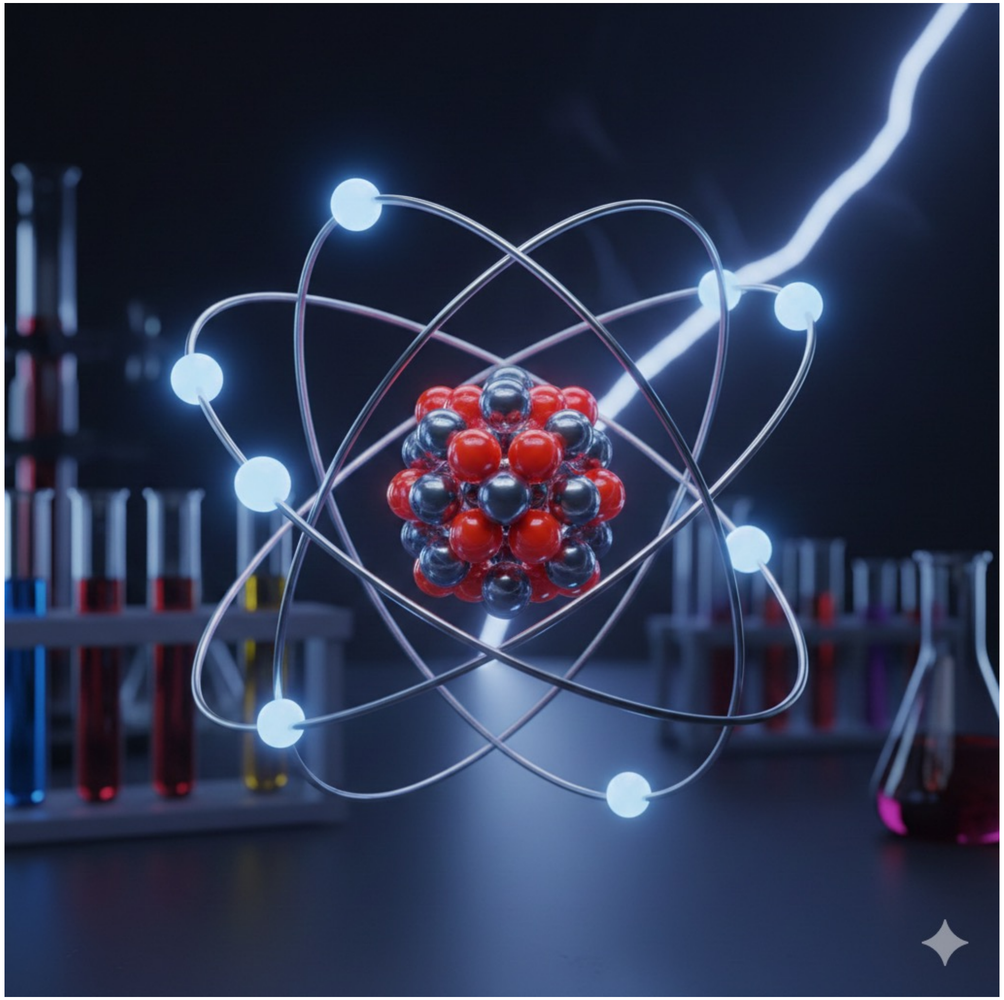
Why we need HPC power



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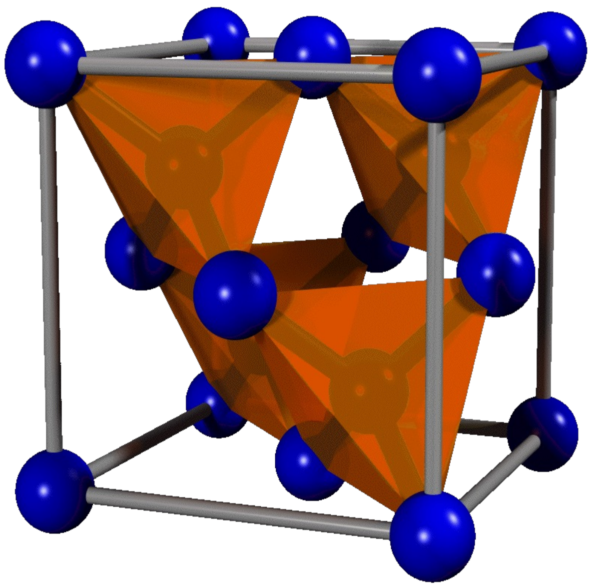
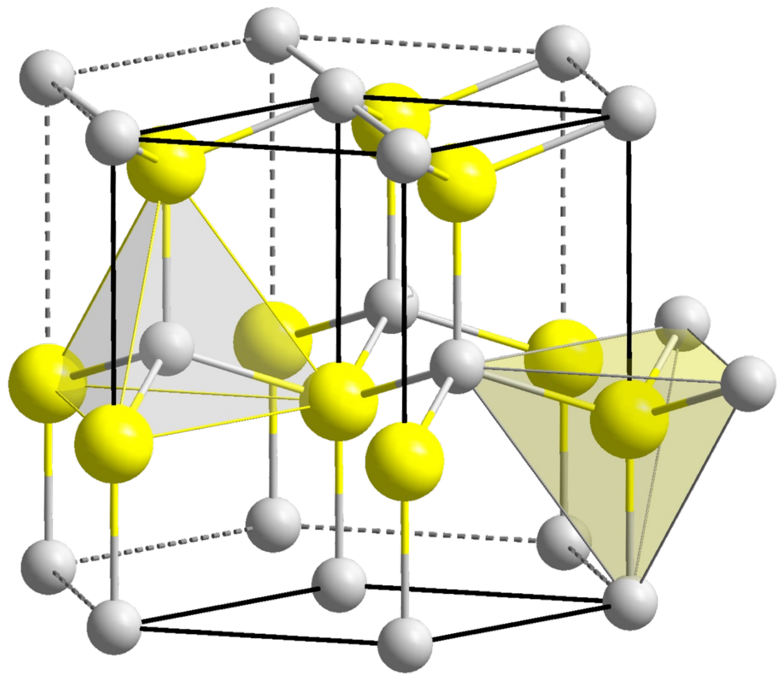
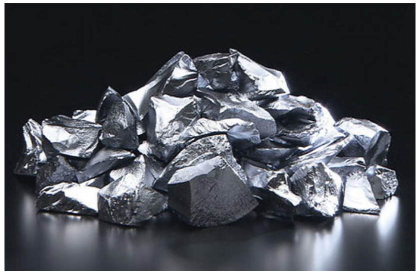
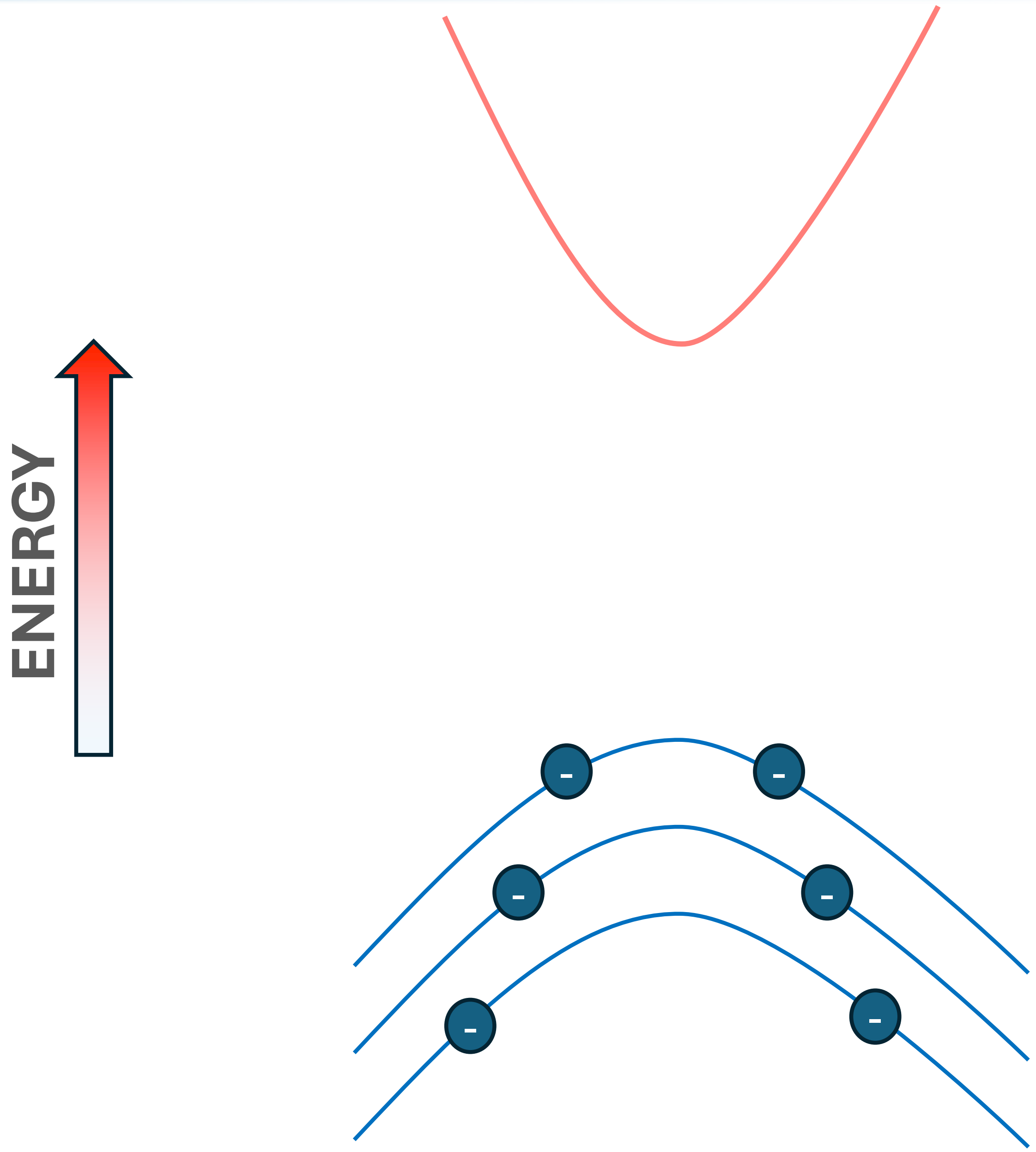


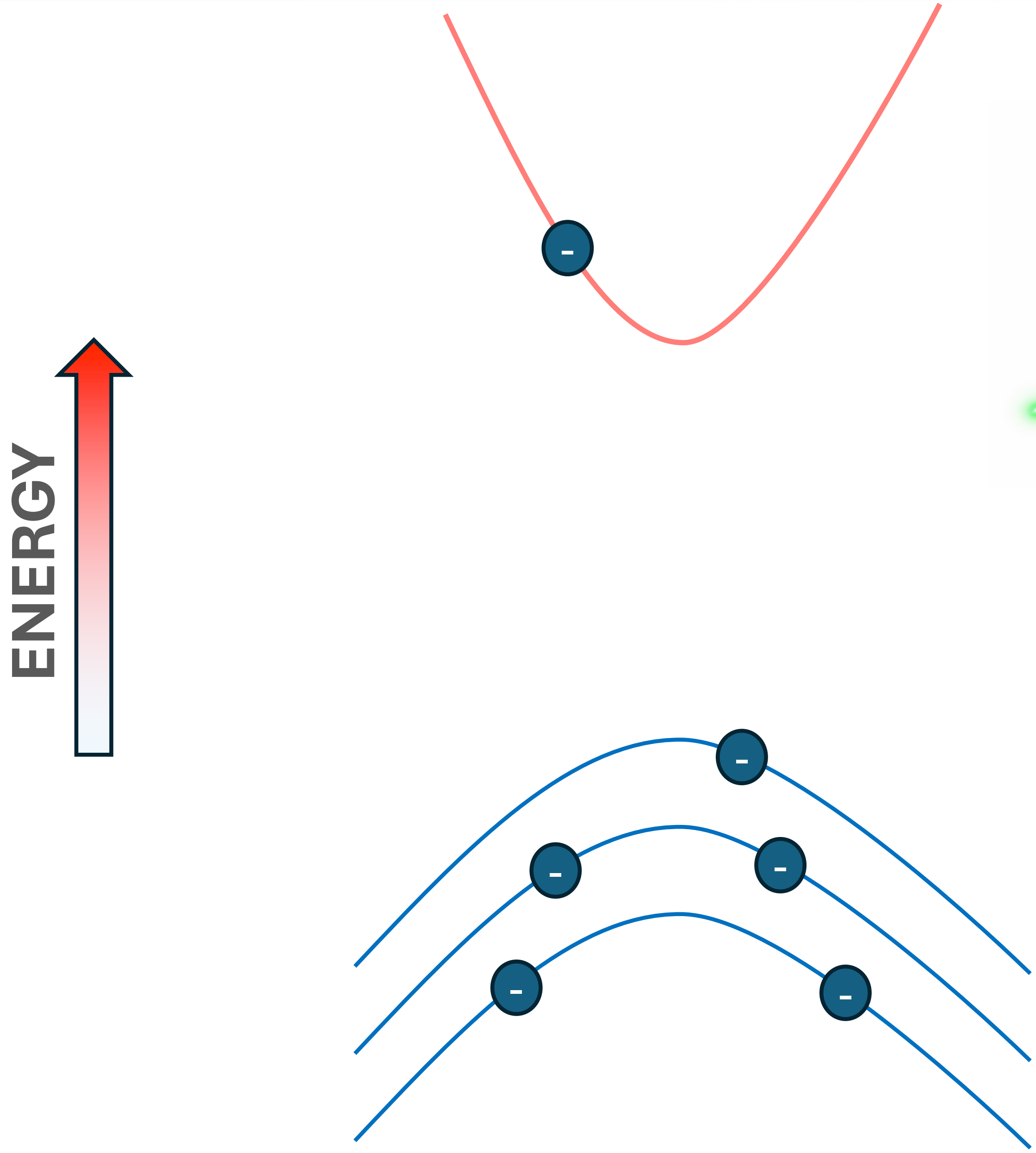


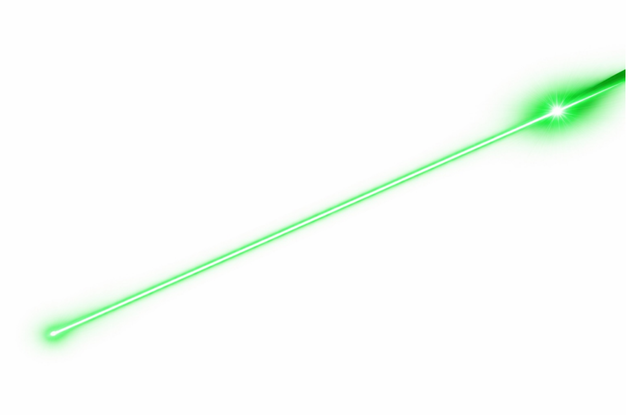


Why we need HPC power



Why we need HPC power





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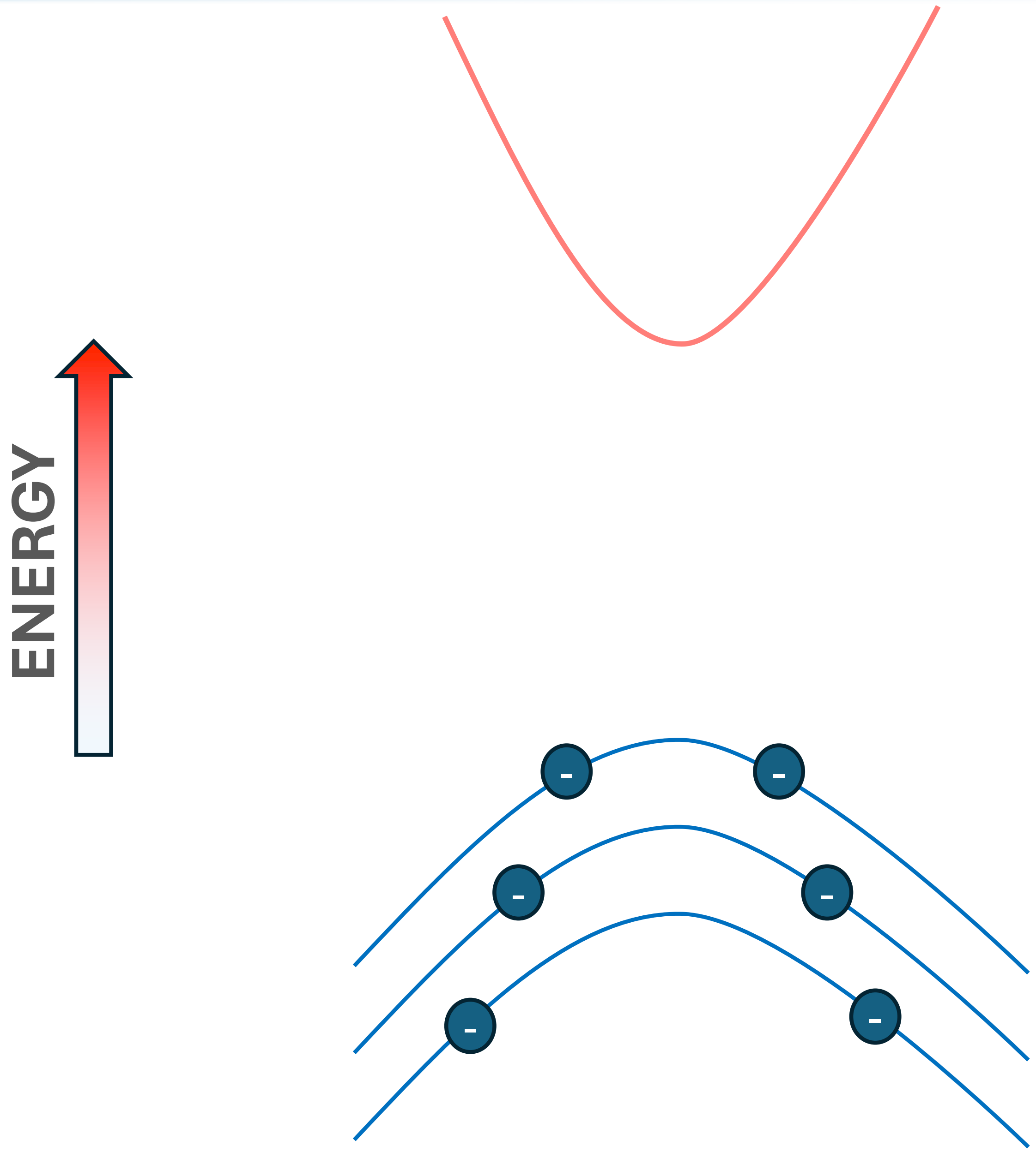

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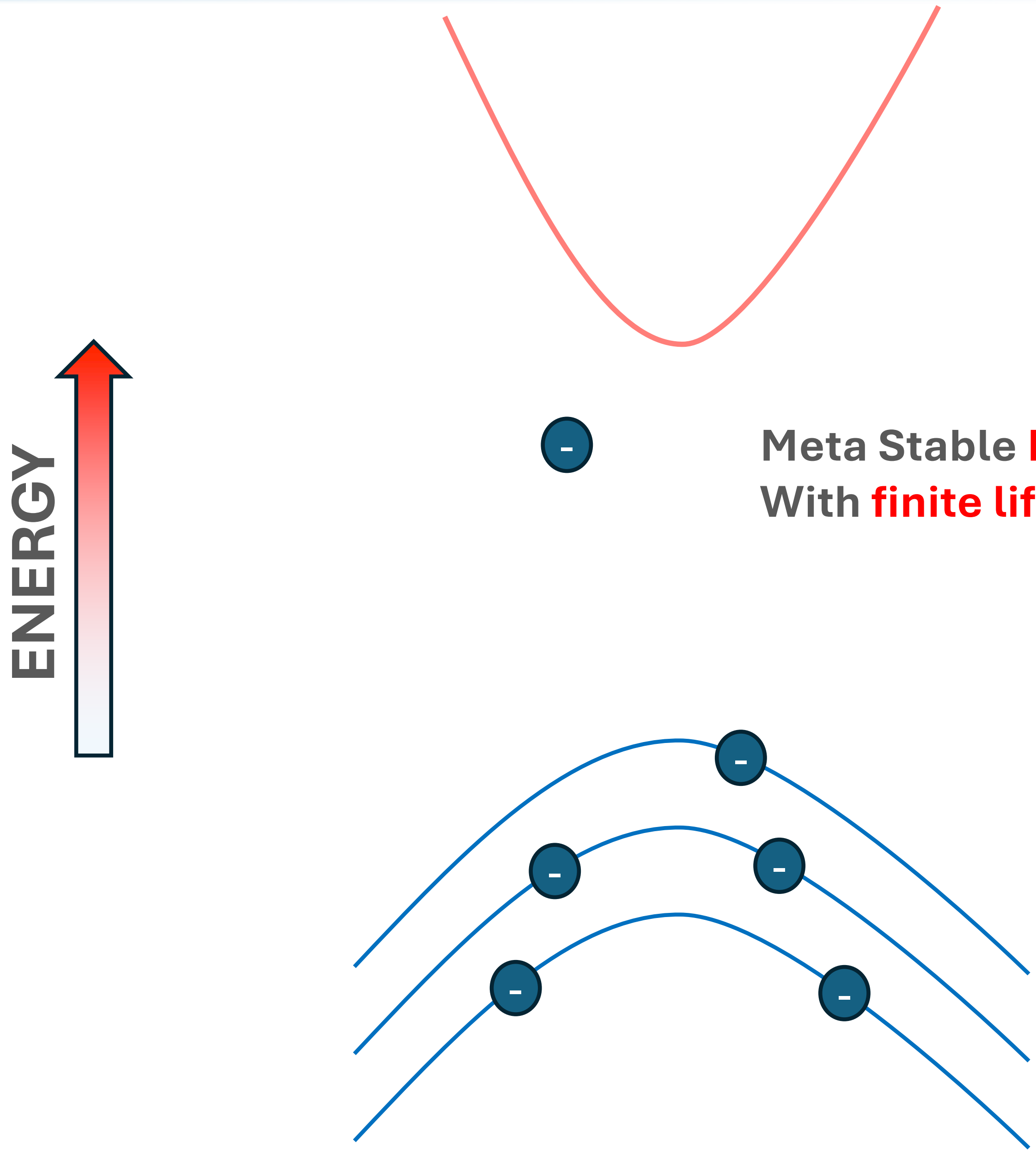
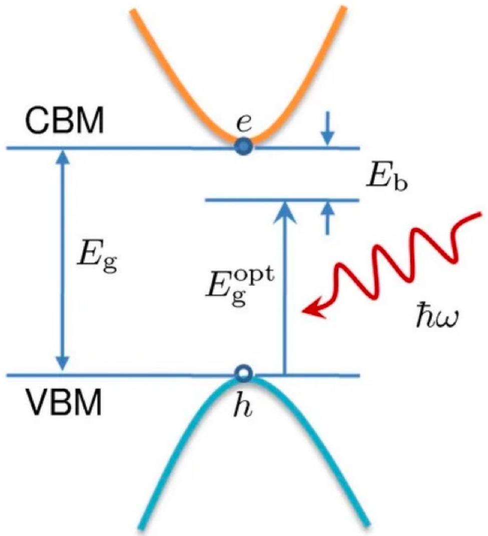
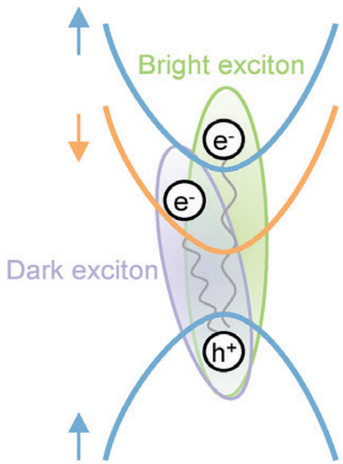


Meta Stable **EXCITON** state
With **finite lifetime**

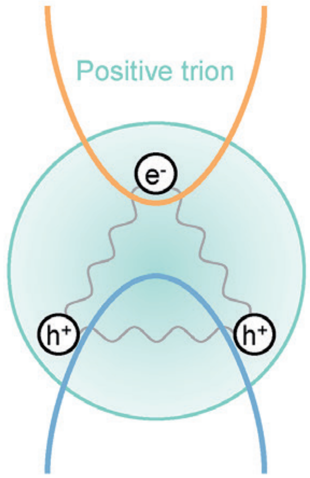
Excitons



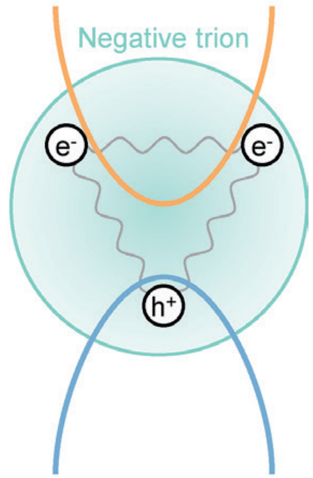
CBM
e
E_b
E_g
$E_\mathrm{g}^\mathrm{opt}$
$\hbar\omega$
VBM
h



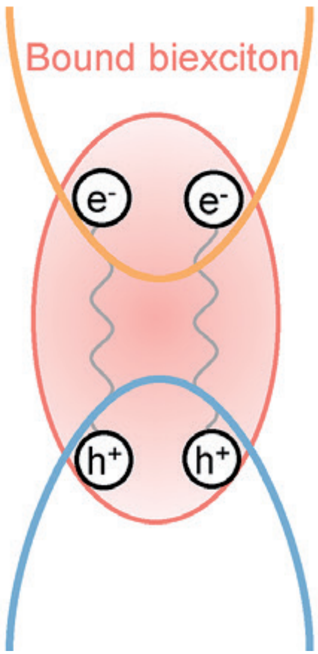
Bright exciton
Dark exciton
e-
e-
h+



Positive trion
e-
h+
h+



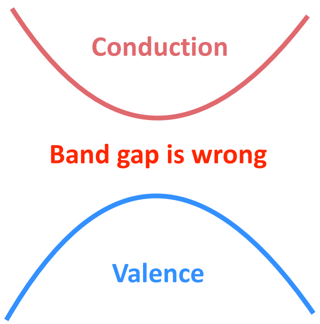
Negative trion
e-
e-
h+



Bound biexciton
e-
e-
h+
h+

Excitons

Density Functional Theory



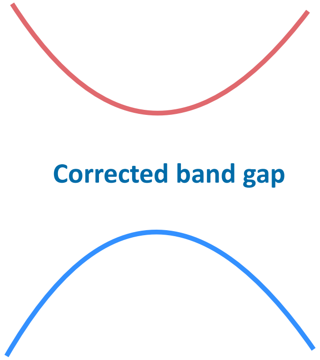
Effective single particle systems

$$\left(-\frac{1}{2}\nabla^2 + V_{Ext} + V_H + V_{XC}\right)\Phi_i = E_i\Phi_i$$

Independent Particle Approximation

$$\mathrm{Im}(\varepsilon_M(\omega)) \sim \lim_{q\to 0}\sum_{cvk}\left|\langle ck|p|vk\rangle\right|^2 \delta(E(c)-E(v)-\hbar\omega)$$

GW calculations



Correct e-e interaction

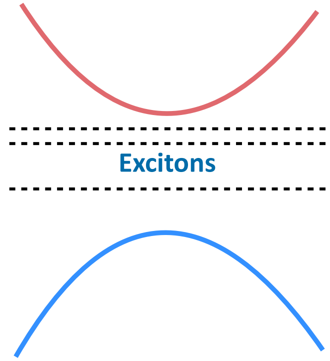
$$\left(-\frac{1}{2}\nabla^2 + V_{Ext} + V_H + \boxed{V_{XC}}\right)\Phi_i = E_i\Phi_i$$

$$\Sigma = iGW$$

Green's function

Screened Coulomb interaction

BSE calculations



$$H_{BSE} = \big(E(c)-E(v)\big)\delta_{vv'}\delta_{cc'}\delta_{kk'} + (2V - W)$$

GW corrected — Exchange — Correlation

$$H_{BSE}A^S_{cvk} = \Omega^S A^S_{cvk}$$

Exciton level

$$\mathrm{Im}(\varepsilon_M(\omega)) \sim \lim_{q\to 0}\sum_{S}\left|\sum_{cvk}A^S_{cvk}\langle ck|p|vk\rangle\right|^2 \delta(\Omega^S-\hbar\omega)$$

Excitons

SCIENCE ADVANCES | RESEARCH ARTICLE

CONDENSED MATTER PHYSICS

Giant enhancement of exciton diffusivity in two-dimensional semiconductors

Yiling Yu[1], Yifei Yu[1], Guoqing Li[1], Alexander A. Puretzky[2], David B. Geohegan[2], Linyou Cao[1,3,4]*

nature nanotechnology

Article https://doi.org/10.1038/s41565-020-01356-9

Excitons in mesoscopically reconstructed moiré heterostructures

ACS NANO

Cite This: ACS Nano 2019, 13, 3500−3511 www.acsnano.org

Coherence and Density Dynamics of Excitons in a Single-Layer MoS_2 Reaching the Homogeneous Limit

nature nanotechnology ARTICLES

https://doi.org/10.1038/s41565-021-00916-1

Check for updates

Electrical tuning of optically active interlayer excitons in bilayer MoS_2

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Probing the Nature of Single-Photon Emitters in a WSe_2 Monolayer by Magneto-Photoluminescence Spectroscopy

nature nanotechnology LETTERS

https://doi.org/10.1038/s41565-020-0750-1

Check for updates

Giant Stark splitting of an exciton in bilayer MoS_2

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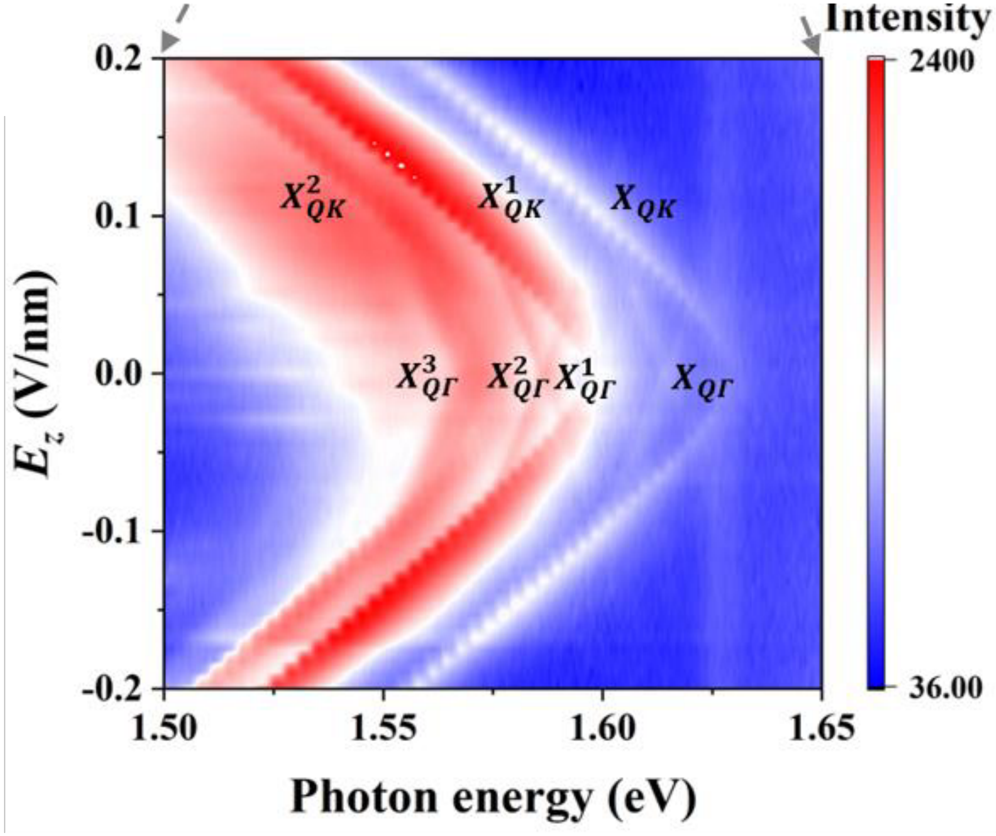
Temperature-Dependent Excitonic Light Manipulation with Atomically Thin Optical Elements

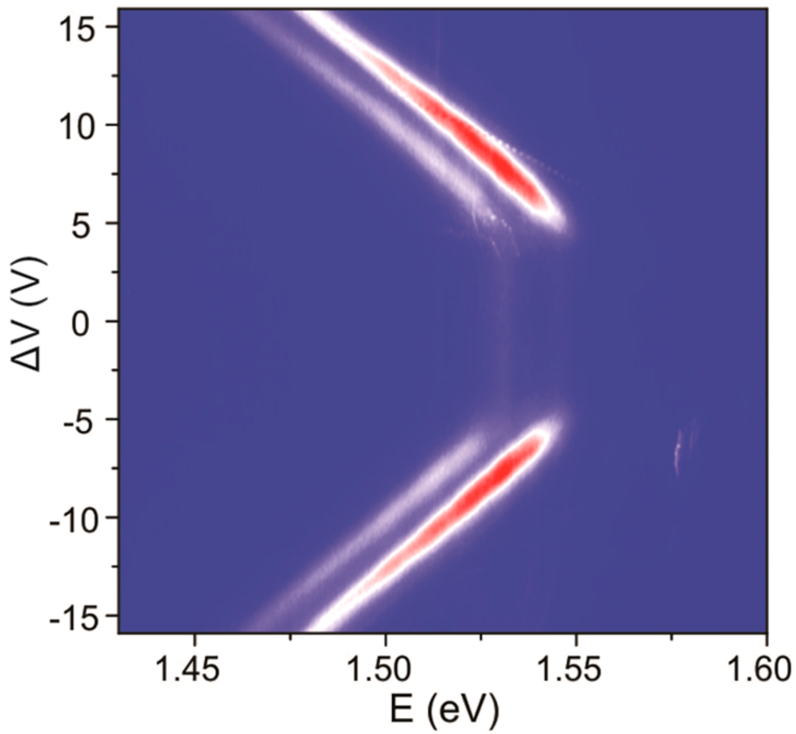
nature nanotechnology

Article https://doi.org/10.1038/s41565-023-01438-8

Ultrafast exciton fluid flow in an atomically thin MoS_2 semiconductor

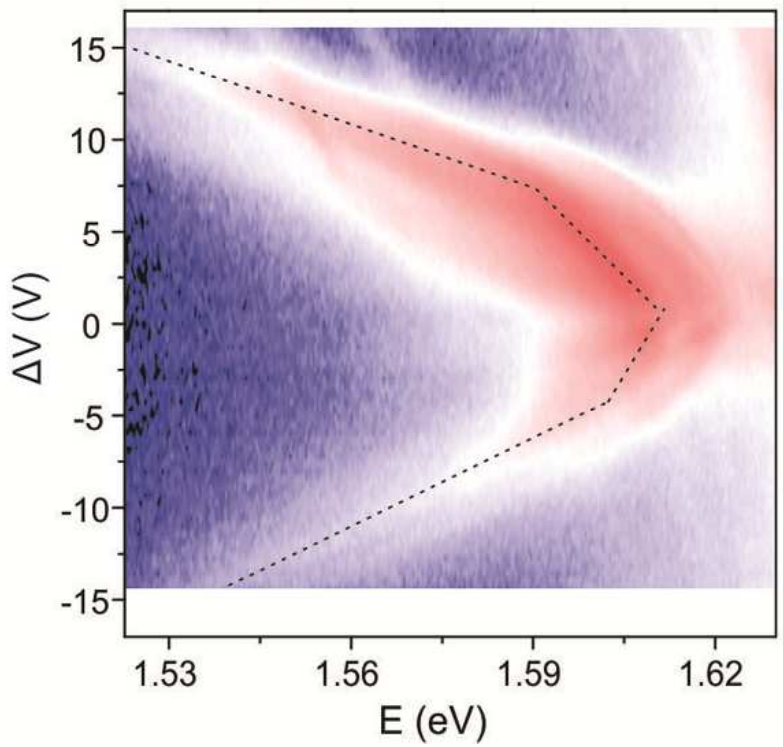
Excitons

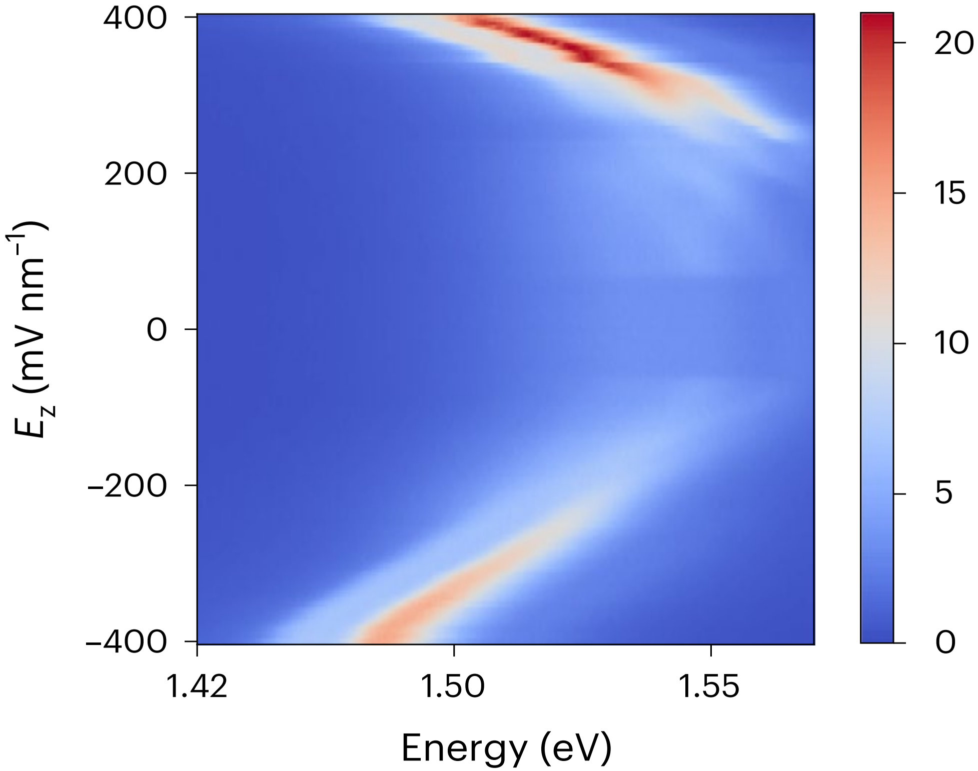




Huang et at. Phys. Rev. B 105 (2022) L041419
Yeh et at. Phys. Rev. B 91 (2015) 041407
Park et at. 2D Mater. 5 (2018) 025003
Wilson et al. Sci. Adv. 3 (2017) e1601832
Nano Lett. 2018, 18, 1, 137–143
Nature Photonics volume 17, pages 615–621 (2023).

Excitons





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Excitons

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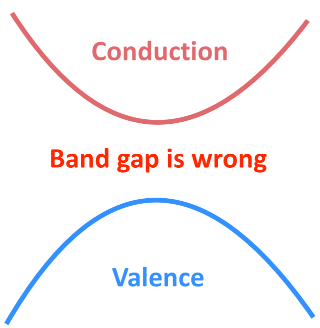

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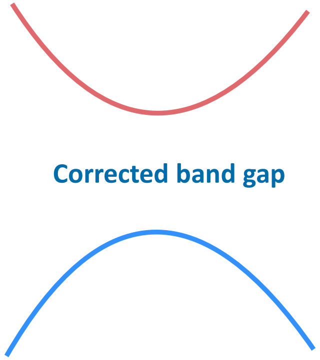

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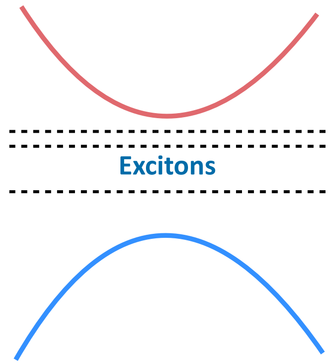

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Exchange

GW corrected

Correlation

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Exciton level

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22 Different Cases
20 h/case in 2 Tier-1 nodes

22 Different Cases
48 h/case in 6 Tier-1 nodes

22 Different Cases
24 h/case in 6 Tier-1 nodes

22 Different Cases
12 h/case in 1 Tier-1 nodes Post Processing

Excitons

NANO LETTERS
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Letter
State- and Momentum-Dependent Nonlinear Stark Effect of Interlayer Excitons in Bilayer WSe2
Cem Sevik, Engin Torun, Milorad V. Milošević, and Fulvio Paleari
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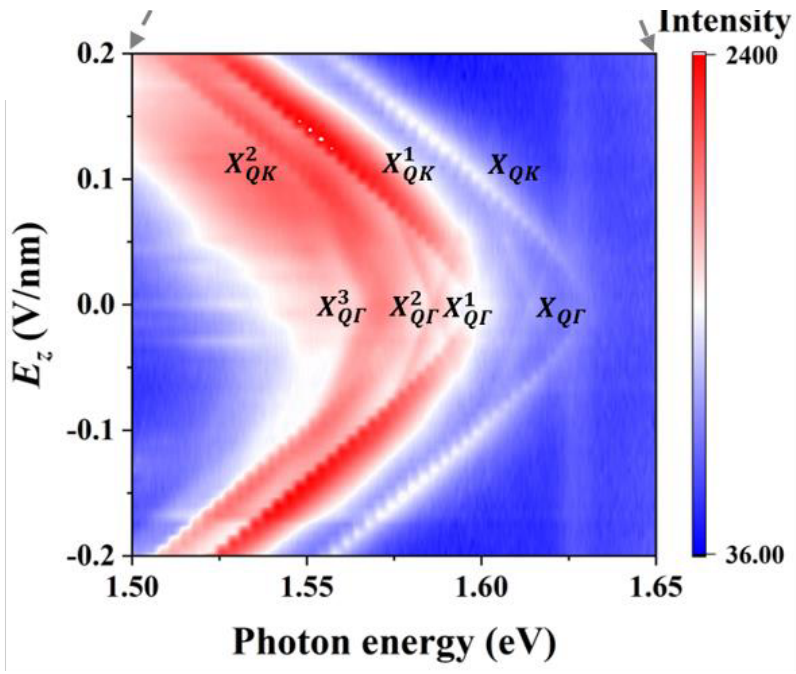
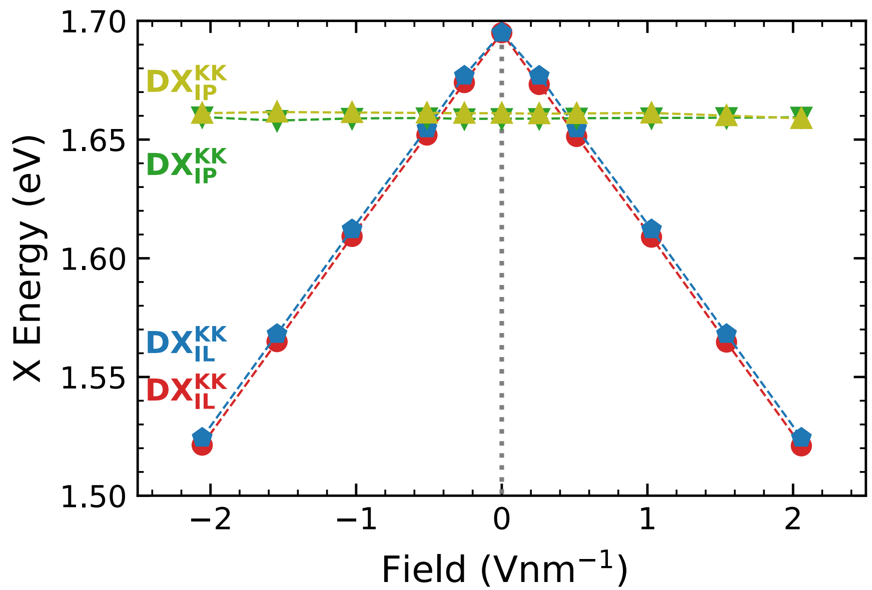
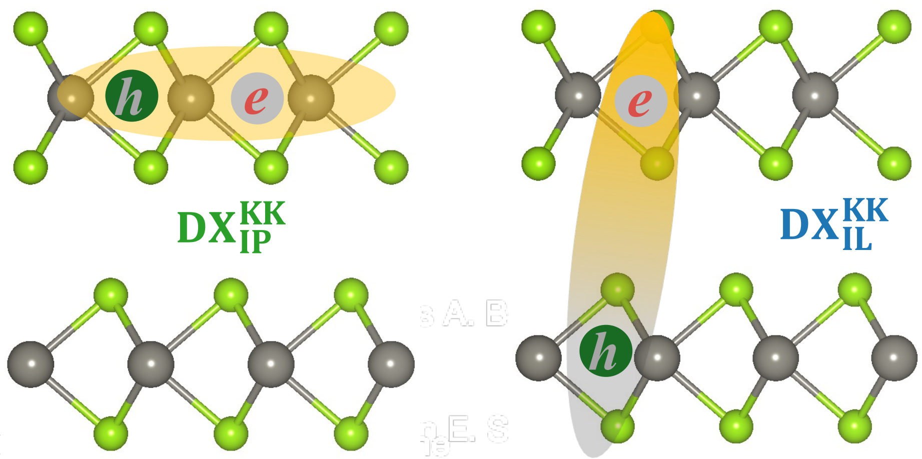


Intensity
2400
36.00
X^2_{QK}
X^1_{QK}
X_{QK}
$X^3_{Q\Gamma}$
$X^2_{Q\Gamma}$
$X^1_{Q\Gamma}$
$X_{Q\Gamma}$
E_z (V/nm)
0.2
0.1
0.0
-0.1
-0.2
1.50
1.55
1.60
1.65
Photon energy (eV)



DX^{KK}_{IP}
DX^{KK}_{IP}
DX^{KK}_{IL}
DX^{KK}_{IL}
X Energy (eV)
1.70
1.65
1.60
1.55
1.50
−2
−1
0
1
2
Field (Vnm^{-1})



h
e
DX^{KK}_{IP}
e
h
DX^{KK}_{IL}

Excitons


NANO LETTERS
pubs.acs.org/NanoLett
Letter

State- and Momentum-Dependent Nonlinear Stark Effect of Interlayer Excitons in Bilayer WSe_2

Cem Sevik,* Engin Torun, Milorad V. Milošević, and Fulvio Paleari*

Cite This: https://doi.org/10.1021/acs.nanolett.5c00682
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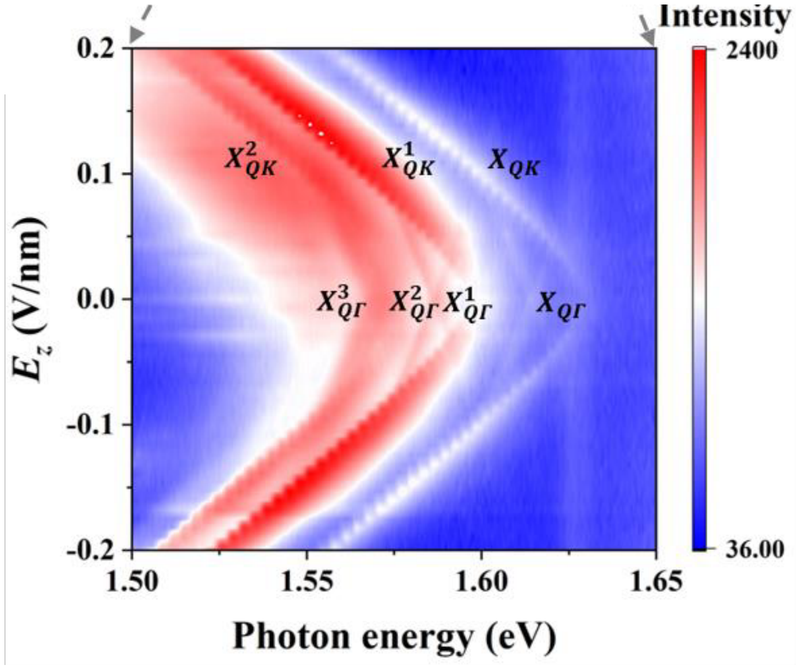
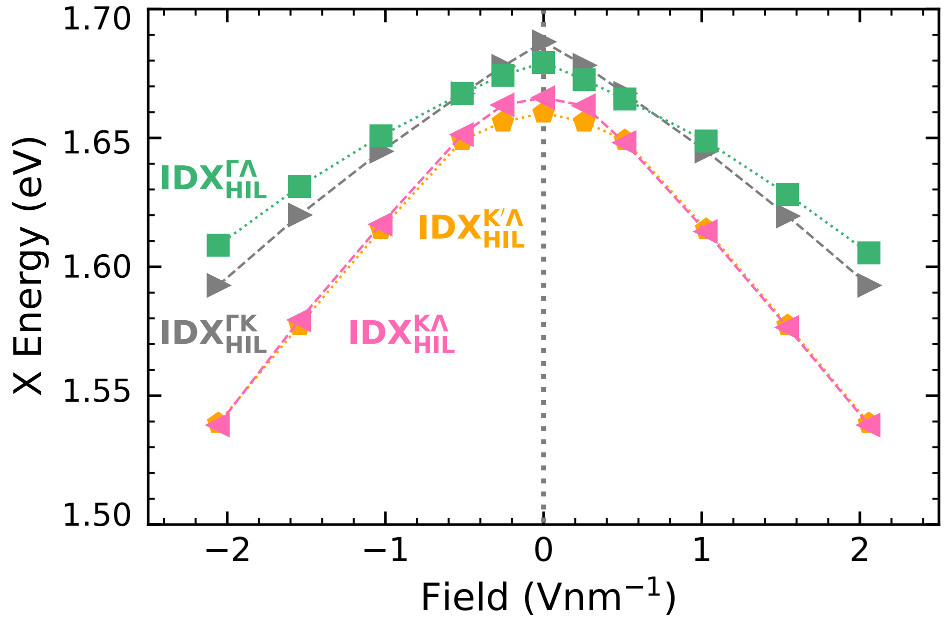
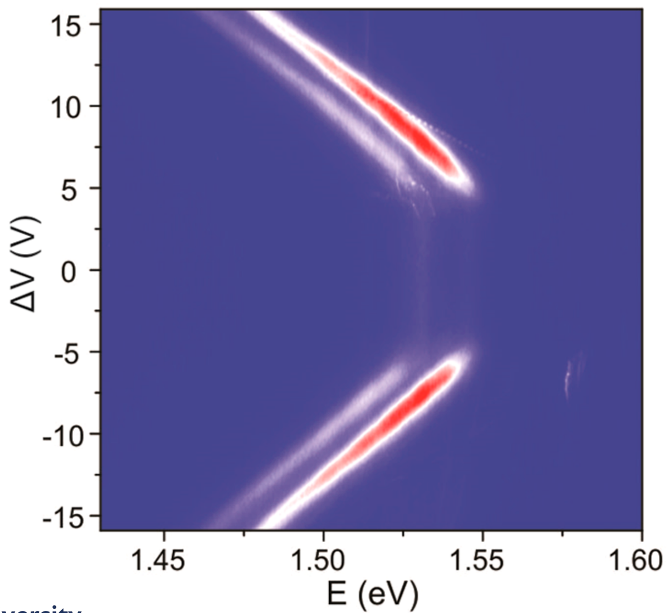
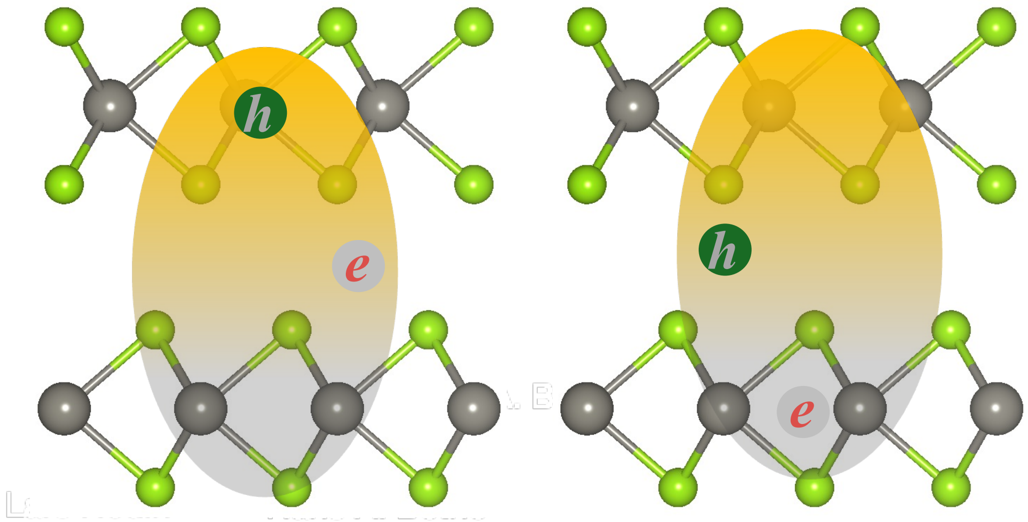




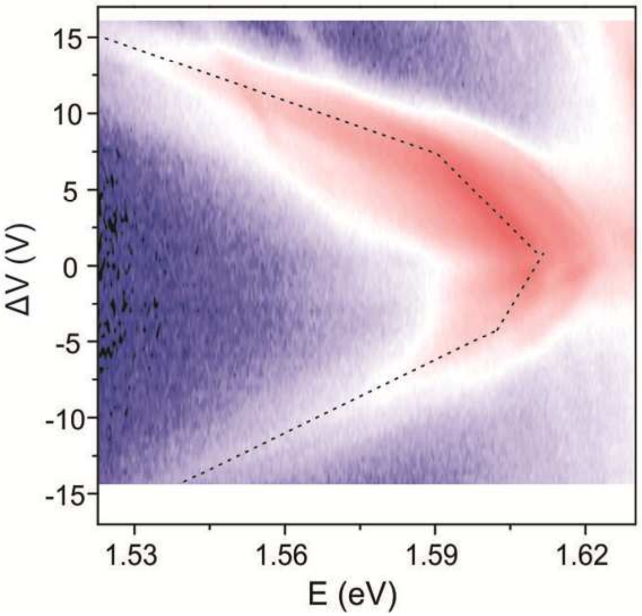


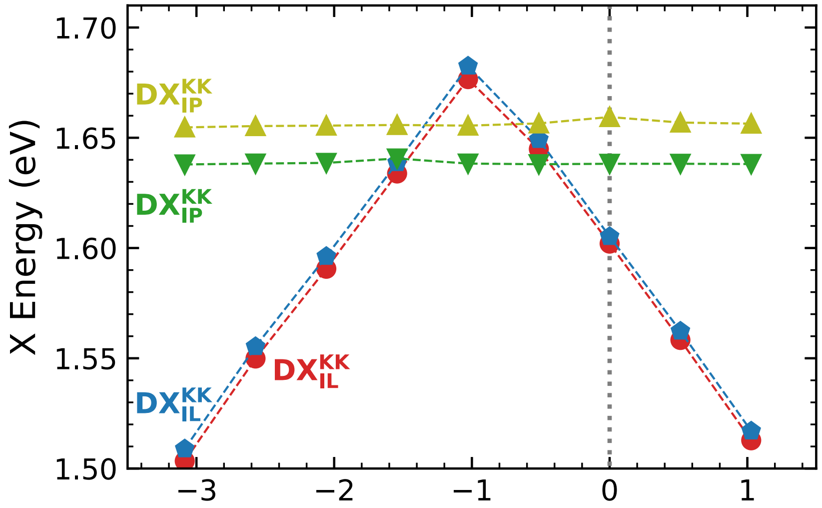


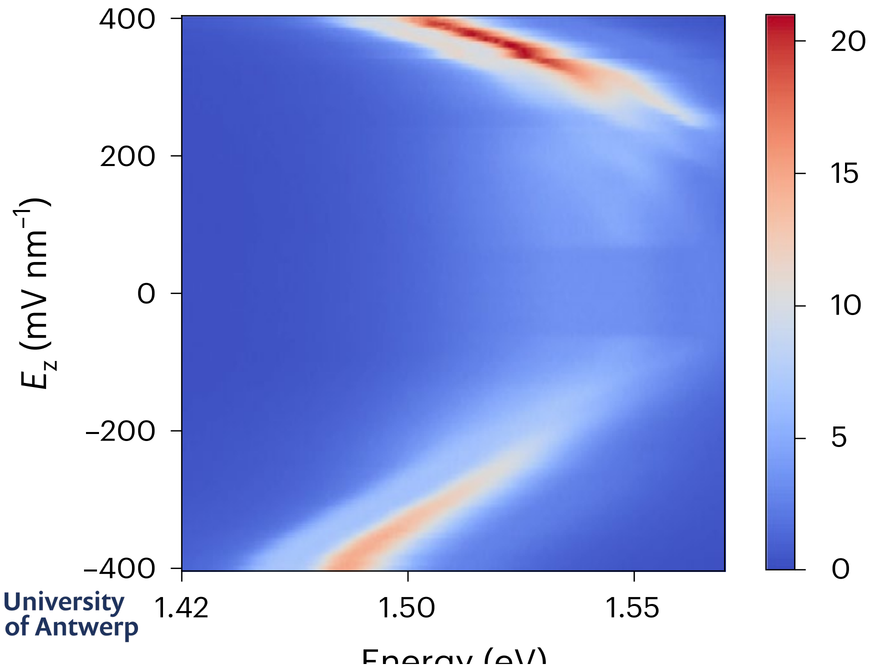
University of Antwerp

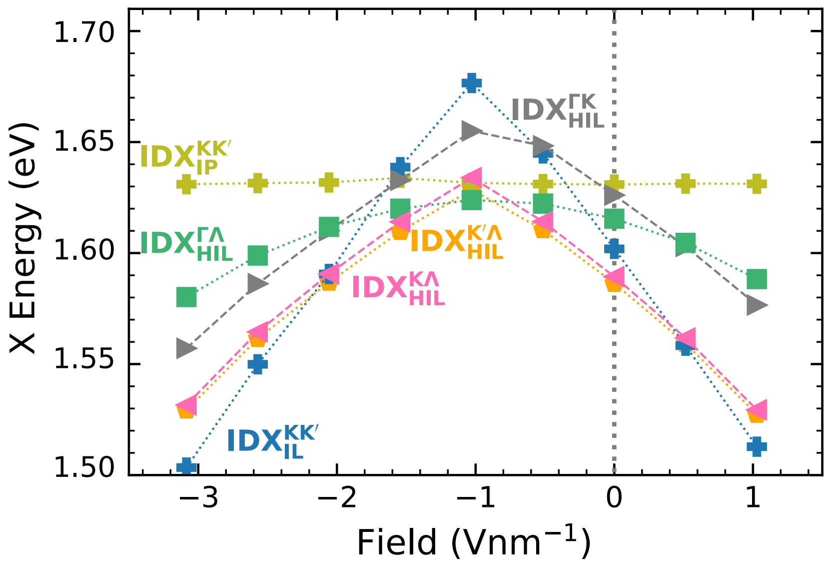
Excitons

AB band structure









Lars Hedin Hans A. Bethe

Excitons

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Cem Sevik,* Engin Torun, Milorad V. Milošević, and Fulvio Paleari*

Cite This: https://doi.org/10.1021/acs.nanolett.5c00682 Read Online

NANO LETTERS
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Intrinsic Control of Interlayer Exciton Generation in Van der Waals Materials via Janus Layers

Engin Torun,*,† Fulvio Paleari,*,† Milorad V. Milošević, Ludger Wirtz, and Cem Sevik*

Cite This: *Nano Lett.* 2023, 23, 3159–3166 Read Online

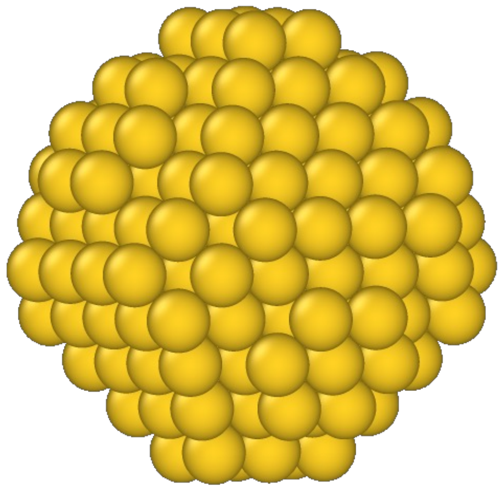
PHYSICAL REVIEW MATERIALS **8**, 075201 (2024)

Optical properties of metallic MXene multilayers through advanced first-principles calculations

Zafer Kandemir,[1] Pino D'Amico,[2] Giacomo Sesti,[2] Claudia Cardoso,[2,*] Milorad V. Milošević,[3,4] and Cem Sevik[3,†]
[1] *Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Istanbul, Turkey*
[2] *CNR-NANO Research Center S3, Via Campi 213/a, 41125 Modena, Italy*
[3] *Department of Physics and NANOlight Center of Excellence, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium*
[4] *Instituto de Física, Universidade Federal de Mato Grosso, Cuiabá, Mato Grosso 78060-900, Brazil*

Why we need HPC power

Machine Learning Interatomic Potentials for Materials



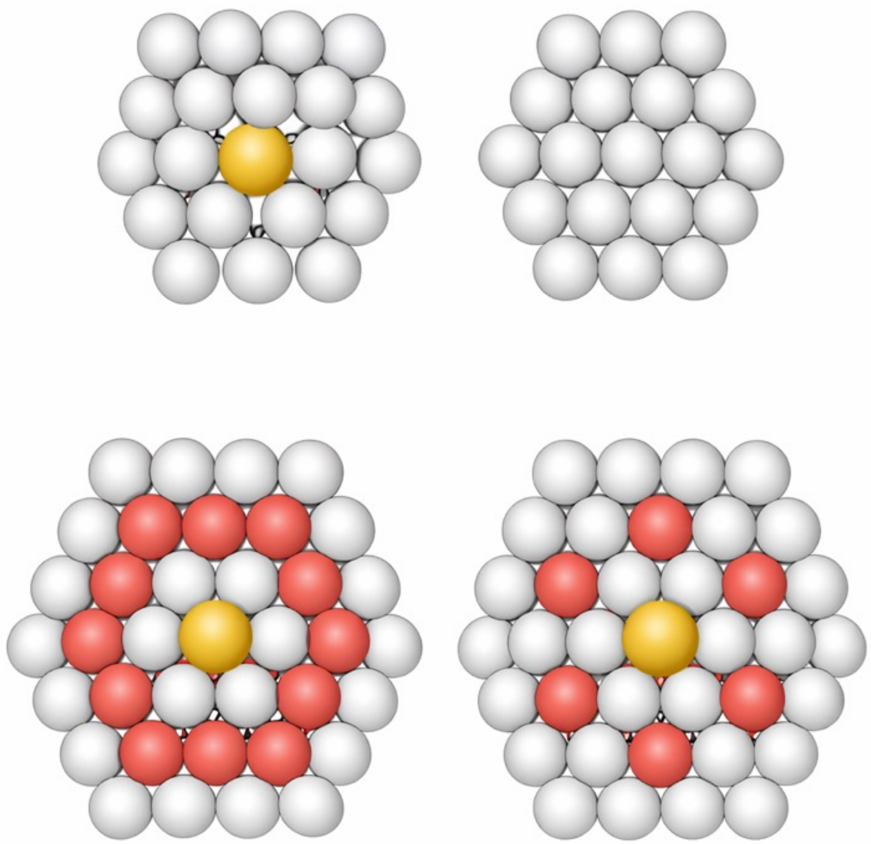
VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

LEONARDO CINECA

LUMI

ML Interatomic Potentials

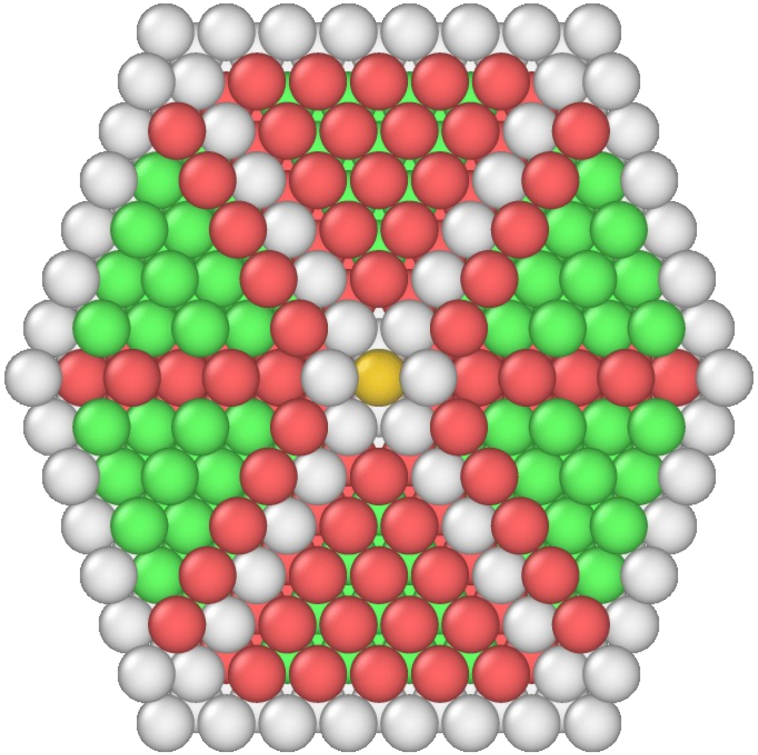


~ 60 Atoms

~ 150 Atoms

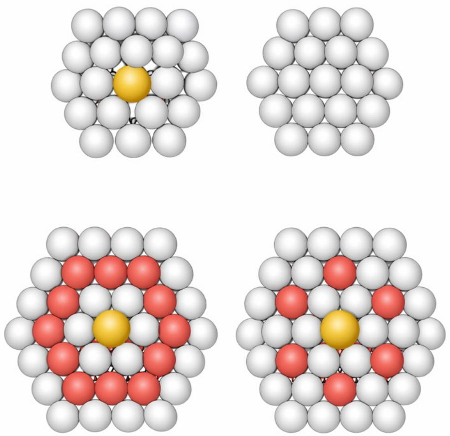
ML Interatomic Potentials

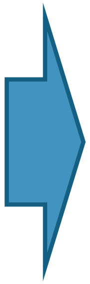
~ 1600 Atoms



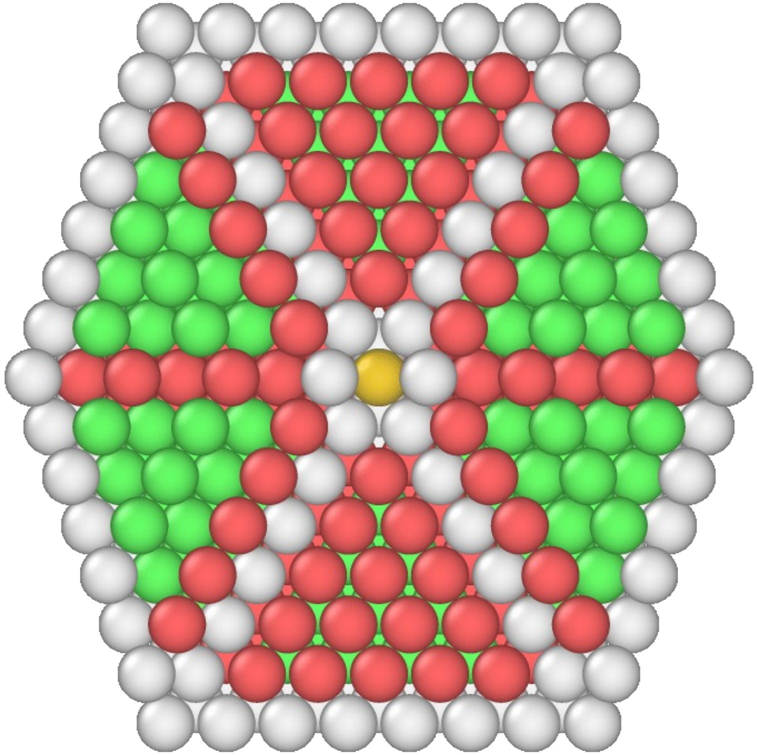
ML Interatomic Potentials

Train ML Potential

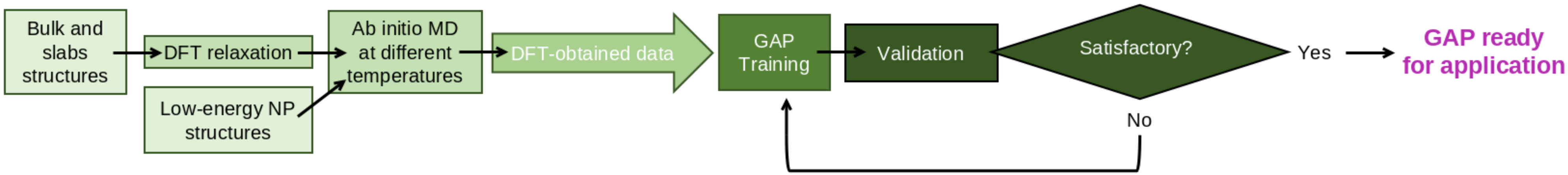


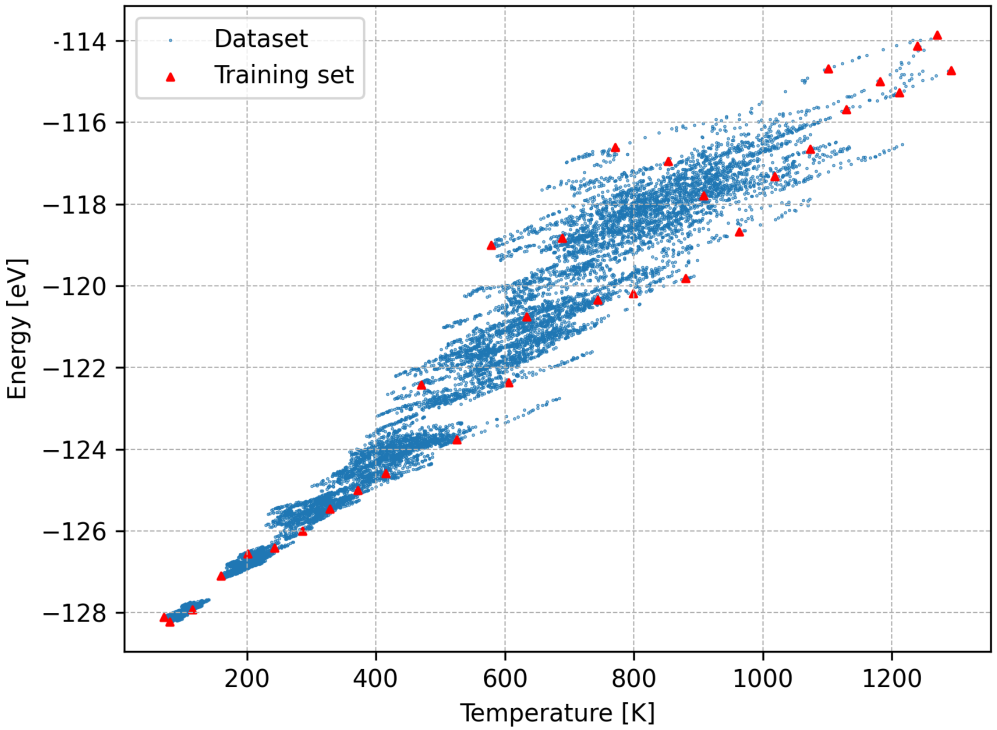


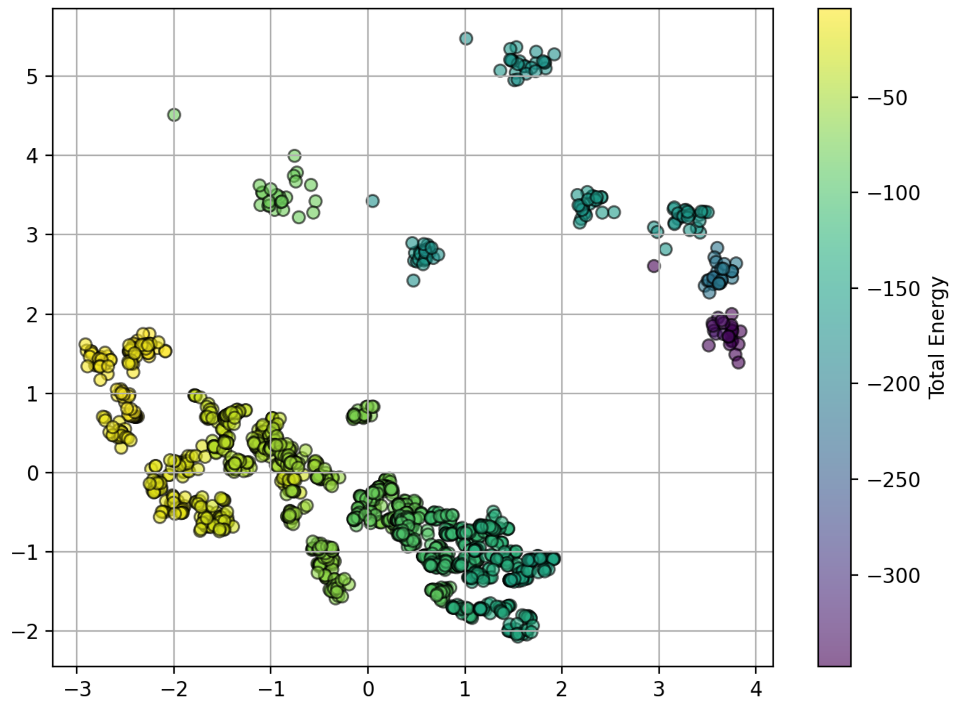
Solve Large Particles



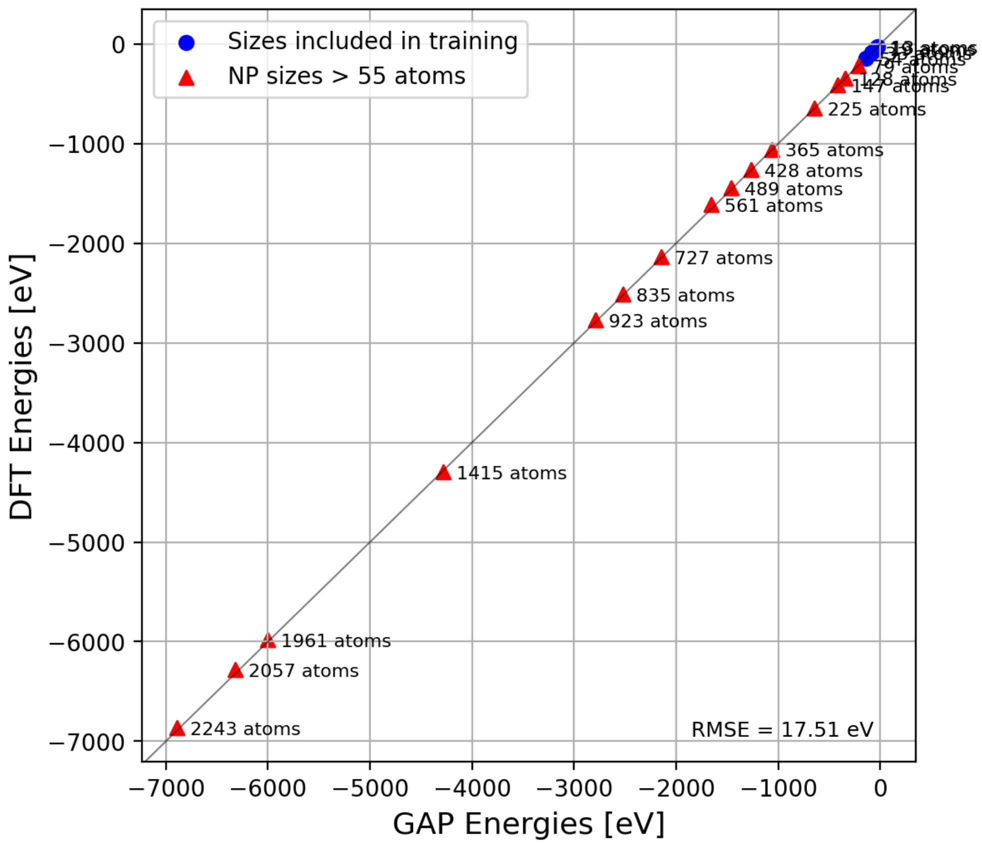
ML Interatomic Potentials

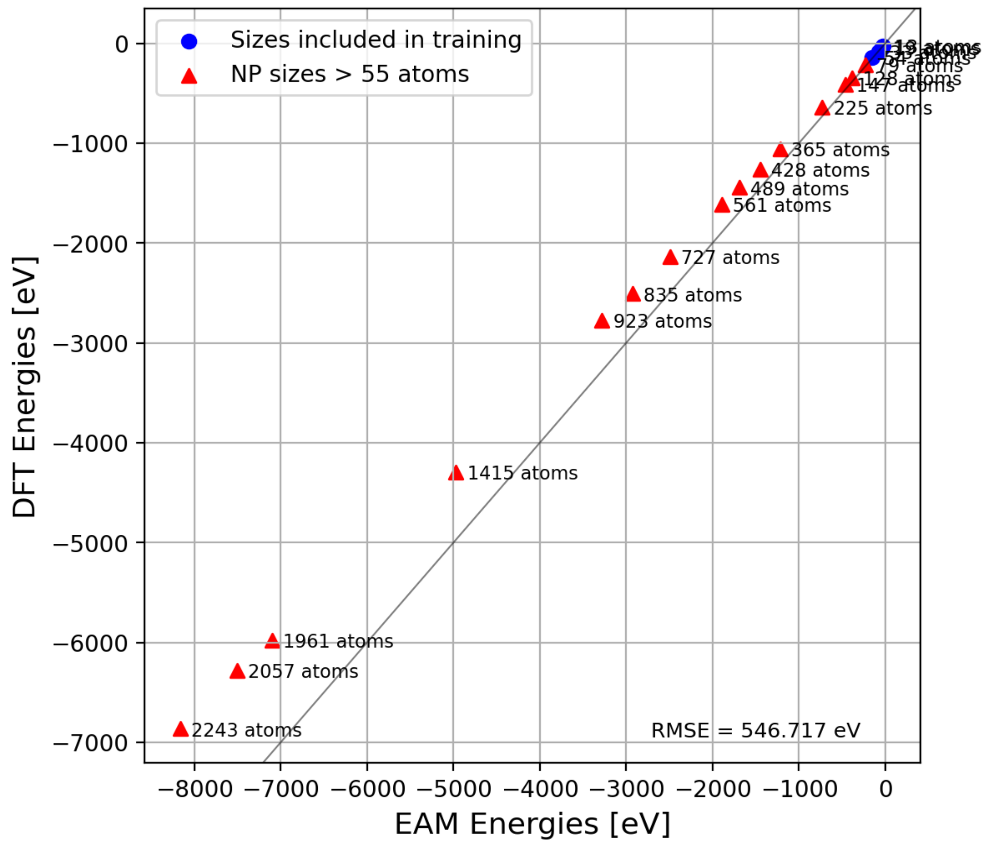




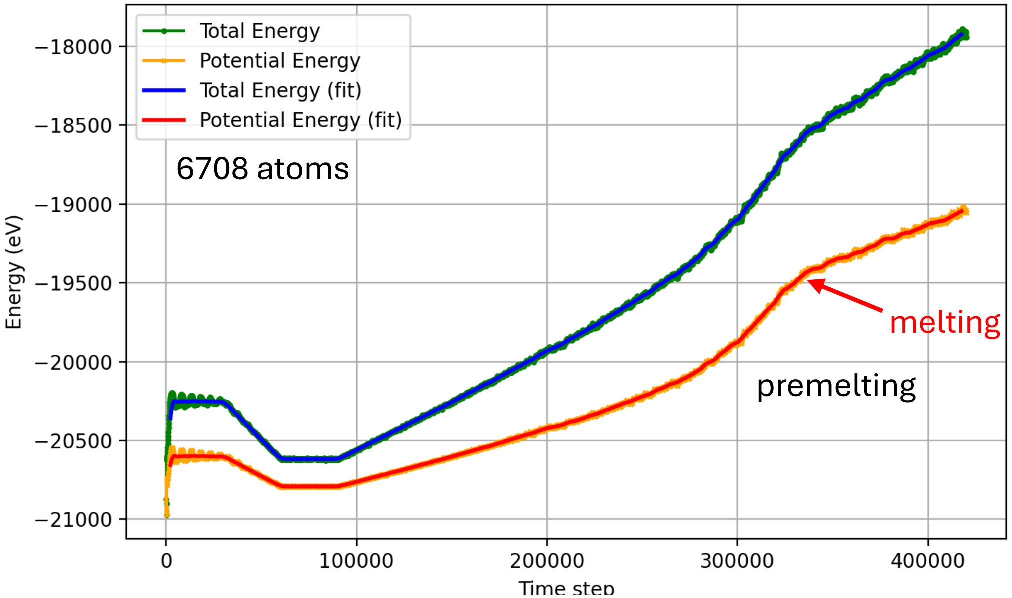


ML Interatomic Potentials





ML Interatomic Potentials



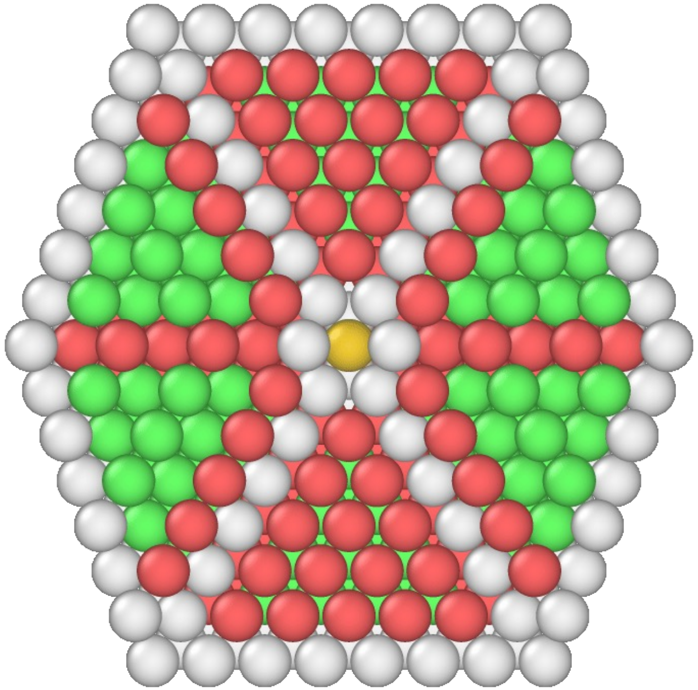


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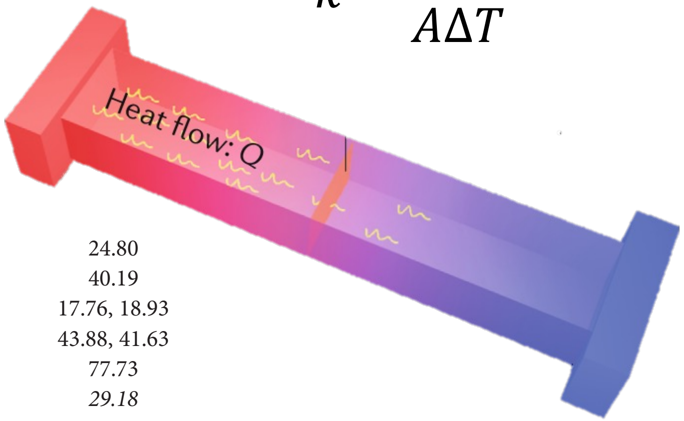
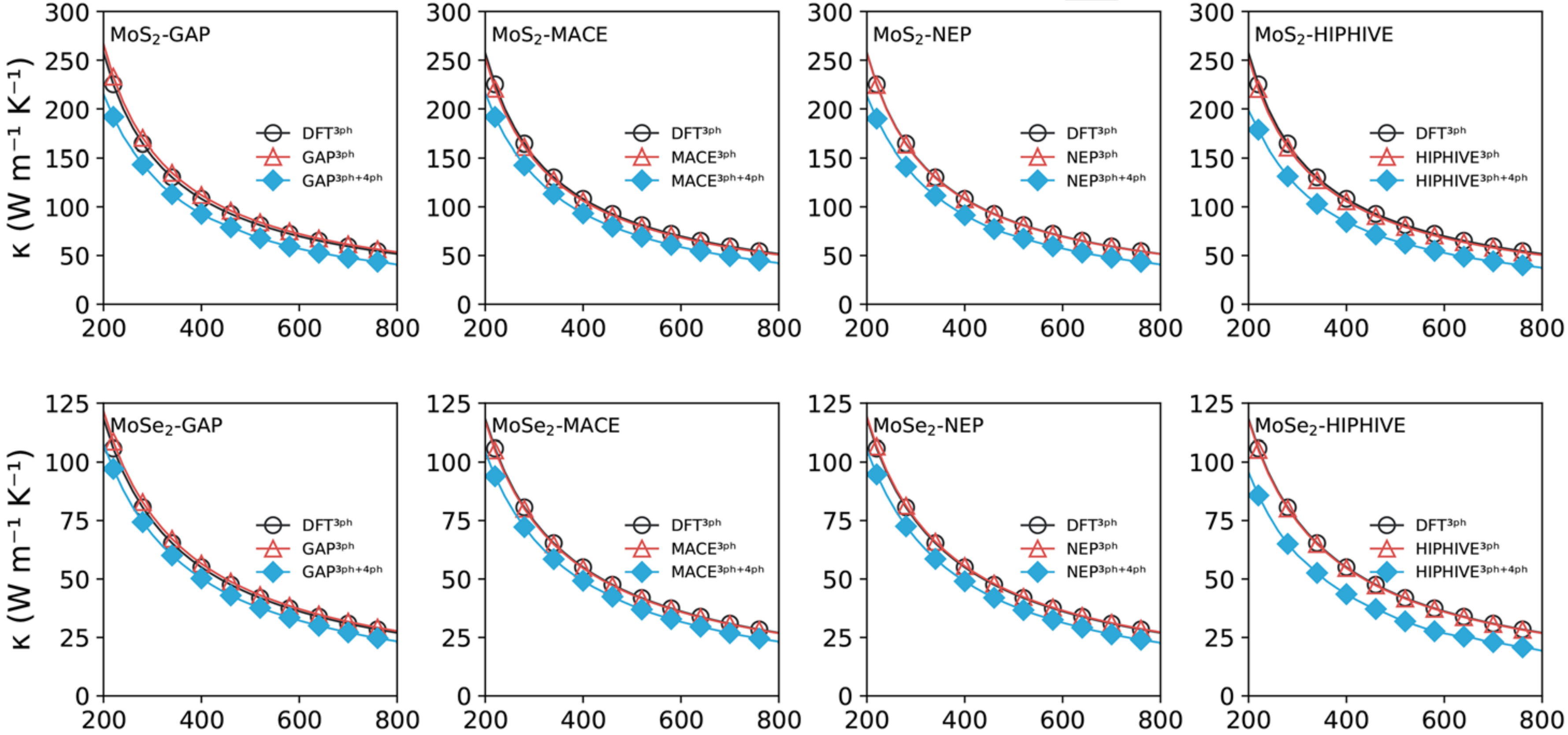
TABLE I. Room-temperature lattice thermal conductivity values of monolayer MoS_2 and $MoSe_2$ collected from the literature, based on first-principles, molecular dynamics, and experimental studies. All reported values have been rescaled according to the out-of-plane lattice constants used in this work: 6.15 Å for MoS_2 and 6.47 Å for $MoSe_2$. Italicized values indicate that the original source did not provide an explicit out-of-plane lattice constant.

First-principles			
MoS_2		$MoSe_2$	
Method	κ ($Wm^{-1}K^{-1}$)	Method	κ ($Wm^{-1}K^{-1}$)
DFT-BTE[58]	151.36	DFT-BTE[59]	54.13
DFT-BTE[60]	135.20	DFT-BTE[61]	∼ 70
DFT-BTE[62]	130.20	DFT-BTE[63]	∼ 60
DFT-BTE[64]	130.00	DFT-BTE[65]	54
DFT-BTE[65]	103.00	DFT-BTE[66]	46.2
DFT-BTE[67]	81.42	DFT-DFPT-Slack Model[68]	17.6
DFT-BTE[59]	89.56		
DFT-DFPT-NEGF[69]	24.52		
DFT-BTE (3^{ph}, $3^{ph}+4^{ph}$)[70]	133.5, 27.7		
DFT-BTE[66]	82.2		
DFT-BTE[63]	∼ 75		
DFT-DFPT-Slack Model[68]	33.6		
DFT-DFPT-Umklapp Model[71]	29.2		
Molecular Dynamics			
REBO-LJ-HNEMD[24]	123.66	SW-NEMD[25]	24.80
(SW13, SW13E, SW16)-HNEMD[24]	535.85, 203.98, 290.65	SW-EMD-Green-Kubo[19]	40.19
TB-(EMD-NEMD)[20]	0.97, 1.22	SW-NEMD-(AC, ZZ)[21]	17.76, 18.93
SW-NEMD[25]	32.89	SW-NEMD-(AC, ZZ)[16]	43.88, 41.63
SW-RNEMD-(AC, ZZ)[23]	32.95, 53.91	MLFF-NEP-HNEMD[17]	*77.73*
SW-EMD-Green-Kubo[19]	90.00	SW-SED[22]	*29.18*
SW-EMD-Green-Kubo[18]	116.99		
SW-NEMD-(AC, ZZ)[16]	101.39, 110.26		
SW-NEMD[15]	19.95		
MLFF-NEP-HNEMD[17]	161.62		
SW-SED[22]	89.4		
Experimental			
Raman (Heat Diff. Modeling)[3]	36.46	Mech.Exf.-Raman (vacuum, air)[10]	(20, 250)
Raman (Heat Diff. Modeling)[72]	70.80	Mech.Exf.-Raman[6]	59
CVD-RTD[73]	30		
Mech.Exf.-Raman[6]	84		
CVD-Opt. Mod.[74]	19.8		
CVD-LHD[60]	13.3		
CVD-MJH[12]	24–100		

$$\kappa = \frac{\Delta Q}{A \Delta T}$$



ML Interatomic Potentials



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Gaussian approximation potentials for accurate thermal properties of two-dimensional materials†

Tuğbey Kocabaş, *[a] Murat Keçeli, *[b] Álvaro Vázquez-Mayagoitia *[b] and Cem Sevik *[c,d]

Thermal conductivity limits of MoS_2 and $MoSe_2$: Revisiting high-order anharmonic lattice dynamics with machine learning potentials

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HPC

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LEONARDO CINECA

LUMI

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- YAMBO
- VASP
- ABINIT

Tier – 2

- PWSCF
- YAMBO
- VASP
- ABINIT
- ML

  Ghent (CPU)

  Ghent (GPU)

GPU (LEONARDO)

- PWSCF
- YAMBO

  BSE (Limited)

CPU (LUMI)

- PWSCF
- YAMBO

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- YAMBO	- YAMBO	- YAMBO	- YAMBO	- YAMBO
- VASP	- VASP	BSE (Limited)		Screening
- ABINIT	- ABINIT			GW
	- ML			
	Ghent (CPU)			
	Ghent (GPU)			
12 MONTHS		12 MONTHS	12 MONTHS	

THANK YOU