Two-dimensional materials for next generation non-volatile memories

Jose H Garcia

Senior Researcher

Catalan Institute of Nanoscience and Nanotechnology

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The Catalan Center of Nanoscience and Nanotechnology (ICN2)

ENABLING RESEARCH AREAS

NANOCHARACTERISATION

MODELLING & SIMULATION

NANOMATERIALS & NANOFABRICATION

ARTIFICIAL INTELLIGENCE COMPUTATIONAL PLATFORM

APPLICATION DOMAINS

NANOSOLUTIONS FOR ENERGY-EFFICIENT INFORMATION PROCESSING

NANOSOLUTIONS FOR SUSTAINABLE ENERGY TECHNOLOGIES

NANOSOLUTIONS FOR MEDICINE

Barcelona, Spain

Theoretical and Computational Nanoscience group

Advanced quantum mechanical simulations

- Disordered materials:
  - Amorphous dielectrics
  - Nonvolatile SOT-MRAM
- Topological quantum devices.
- Quantum device simulations

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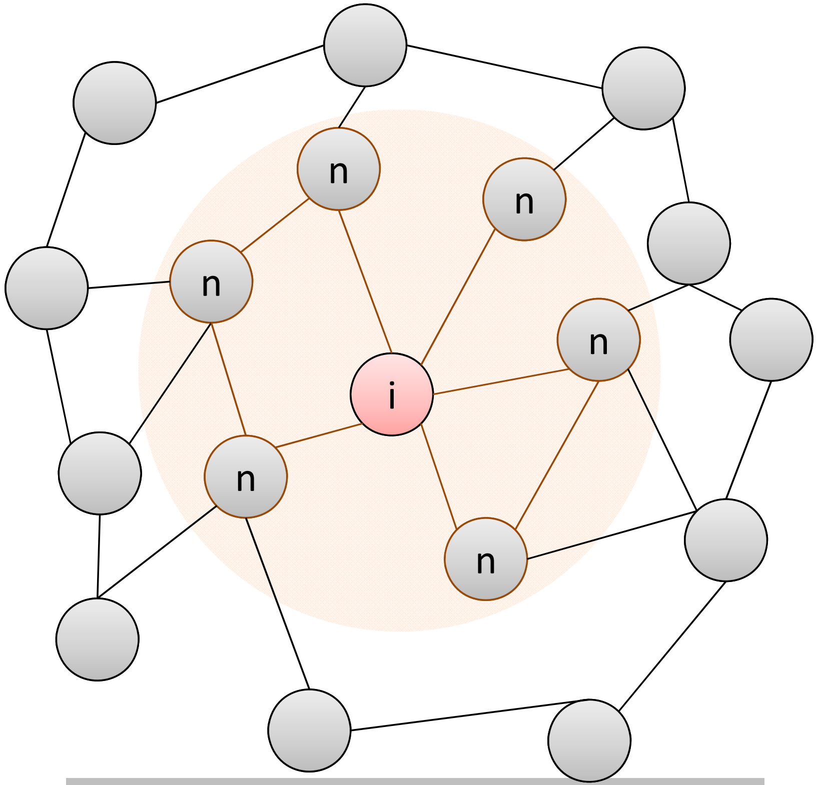
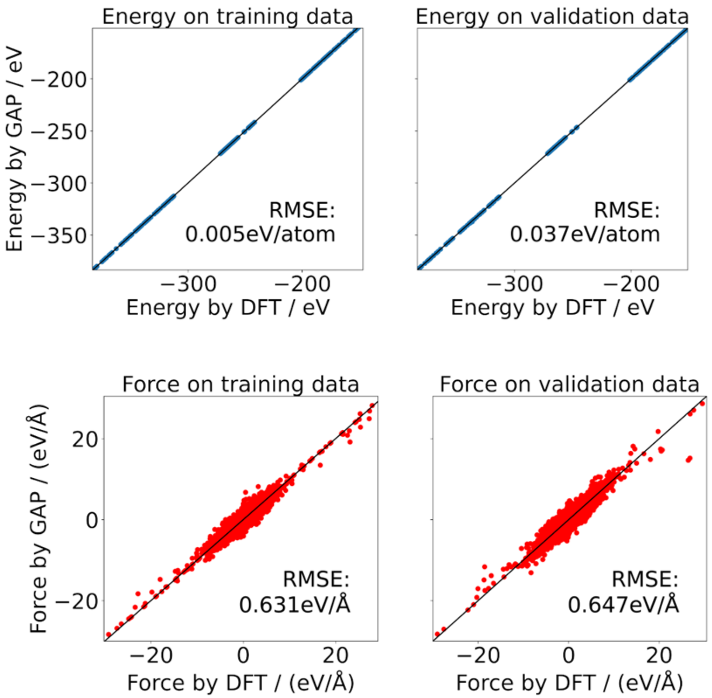
Multiscale data-driven simulations

- Machine learning semiclassical potentials.
- Predictive disordered Hamiltonians.
- Linear-Scaling Quantum Transport simulation: Conductivity, Torkance, Optical absortion, etc.



Local enviroment data-driven methods

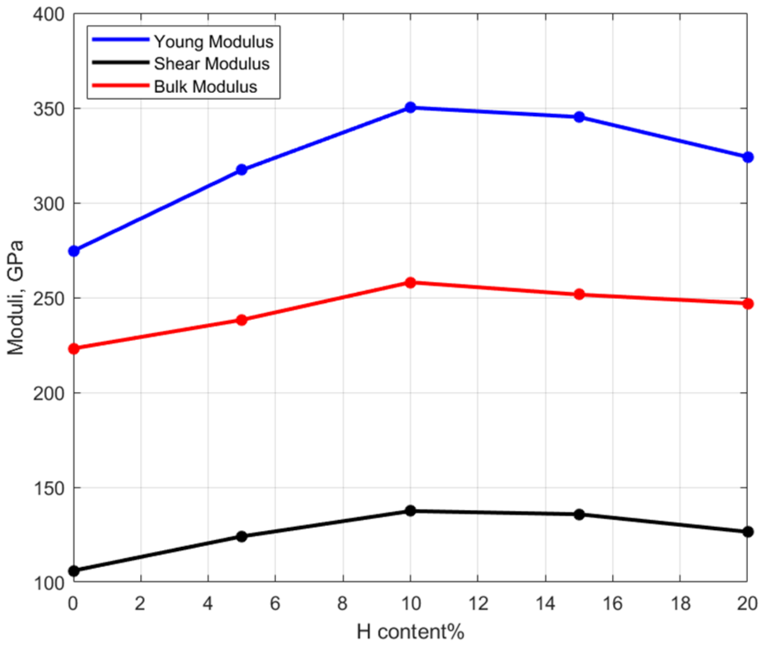


Multiscale data-driven simulations

Experiment (hBN): 865 ± 73 Gpa

Tersoff potential (hBN): 610 ± 22 GPa

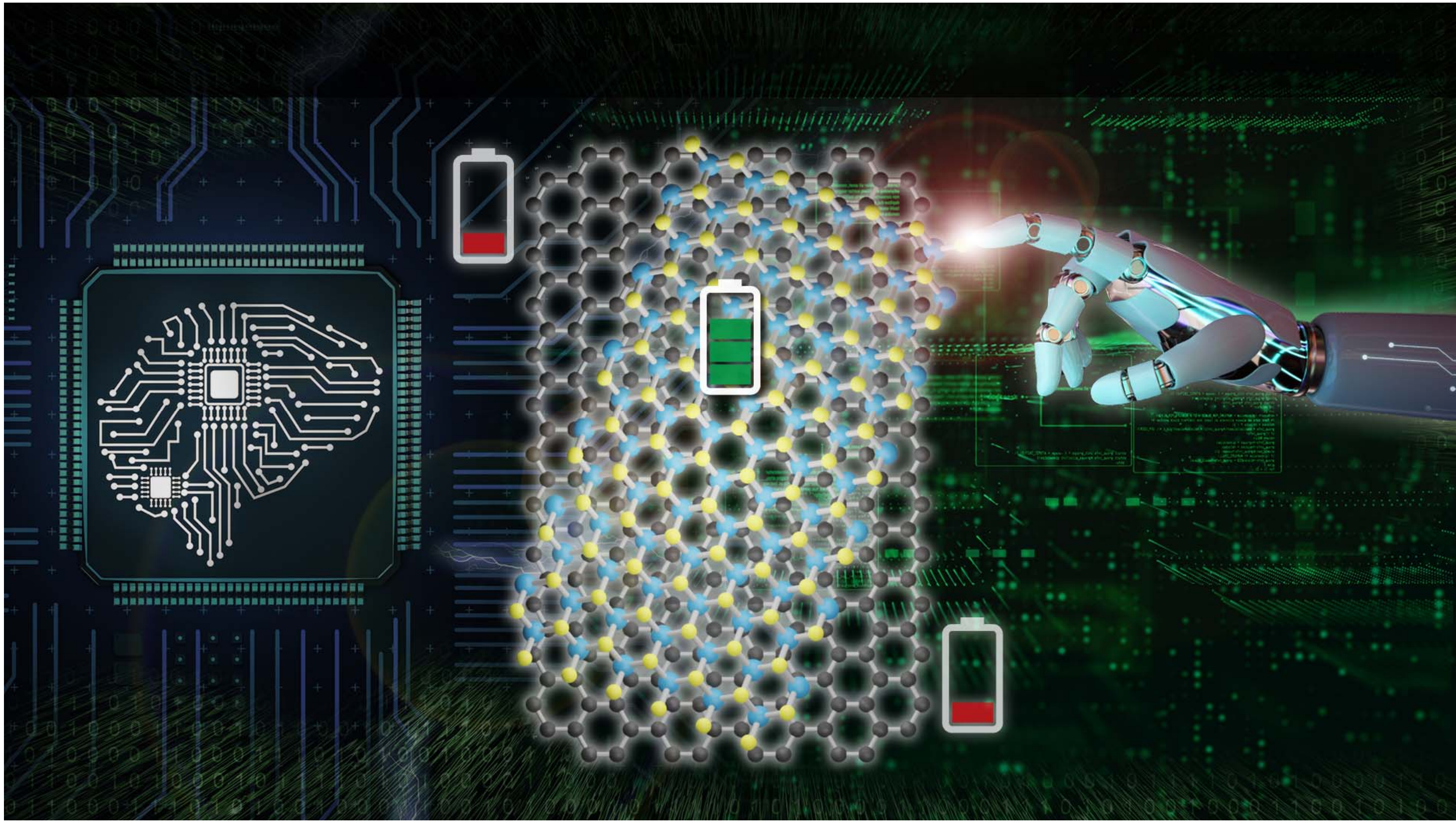
Machine Learning Potential (hBN) 800 ± 15 GPa



Ultralow-dielectric-constant amorphous boron nitride
Seokmo Hong, et al & Hyeon Suk Shin Nature **582**, 511–514 (2020)

ERC-STG: AI4SPIN

Combine heuristic optimization and AI for spin-orbit memories



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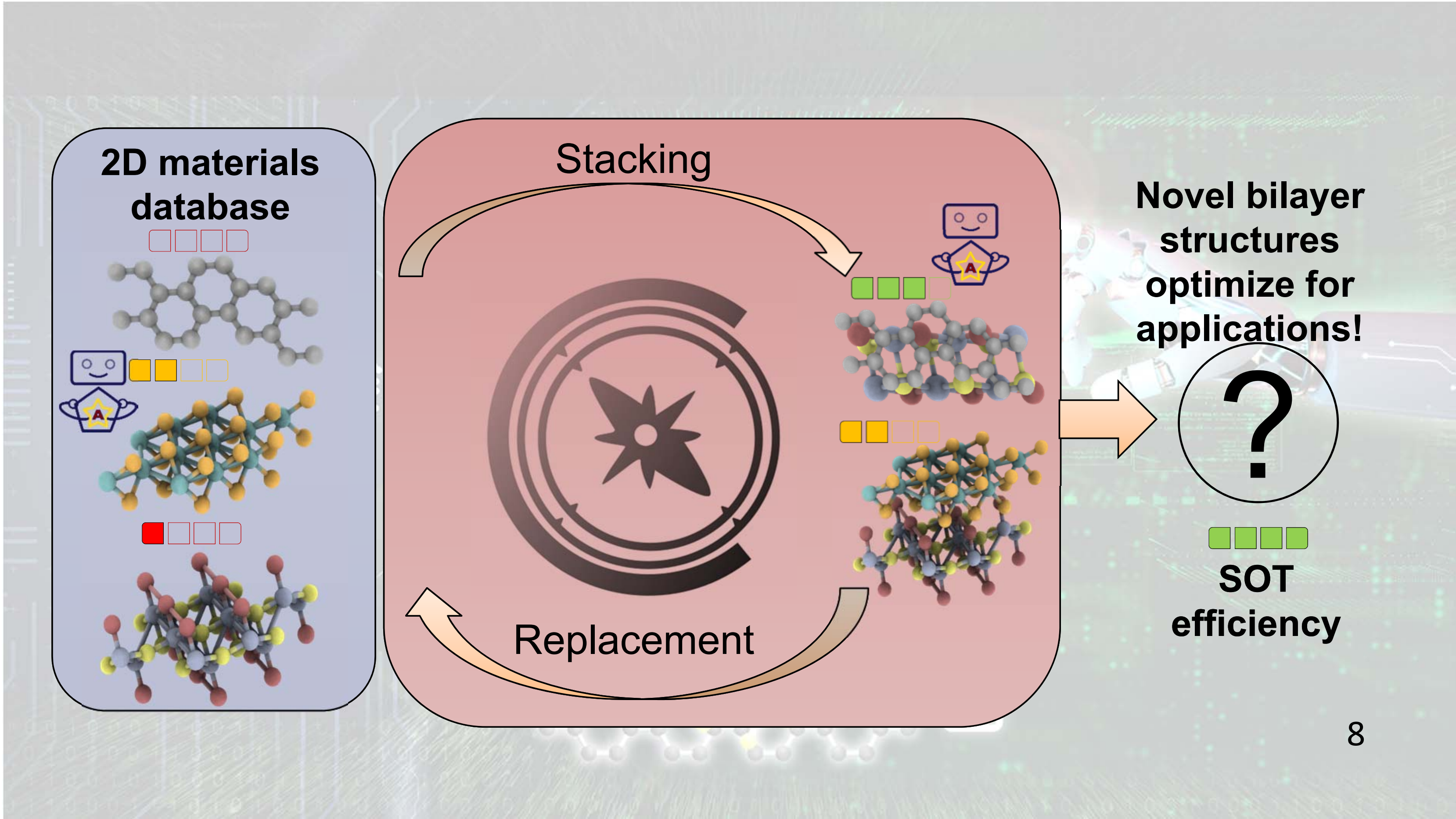


2D materials database

Stacking

Replacement

Novel bilayer structures optimize for applications!

?

SOT efficiency

Linear-scaling quantum transport methodologies

$$\chi^{A}_{\alpha,\beta}(\mu,T) = \int_{-\infty}^{\infty} d\varepsilon\, \mathrm{f}(\mu,\varepsilon,T)\,\mathrm{Tr}\left[\frac{dG^{+}(H,\varepsilon)}{d\varepsilon}A_{\alpha}\mathrm{Im}[G^{+}(H,\varepsilon)]j_{\beta} - \mathrm{Im}[G^{-}(H,\varepsilon)]A_{\alpha}\frac{dG^{-}(H,\varepsilon)}{d\varepsilon}j_{\beta}\right]$$

- A_{α}, j_{β} operator matrices
  H Hamiltonian matrix
- $G^{\pm}(H,\varepsilon)$ Green's functions

$N = 10^{6} - 10^{9}$
atoms

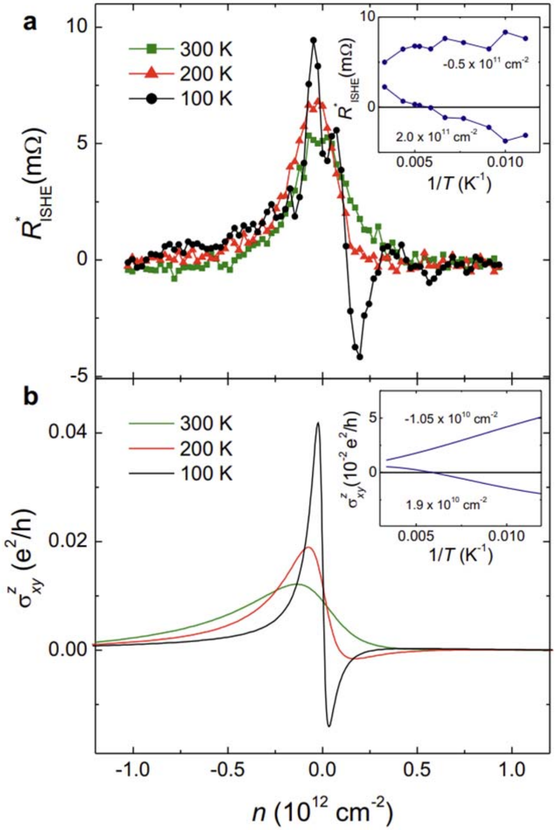
O(N) real-space algorithms

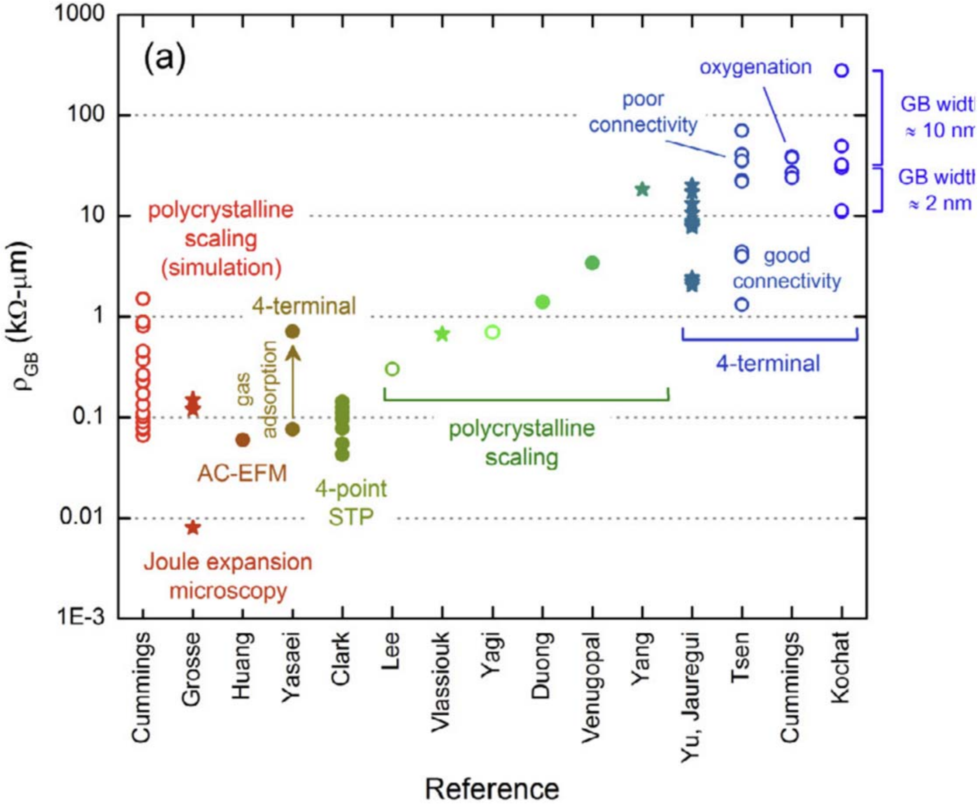
$O(N^{3}) \longrightarrow O(N)$

1 billion years → *1 month*

Z. Fan, Jose H.Garcia, A W. Cummings et al, Physics Reports 903, 7, 1-69 (2021)
Jose H. Garcia, Lucian Covaci, Tatiana G. Rappoport , *Phys. Rev. Lett.* 114, 116602 (2015)

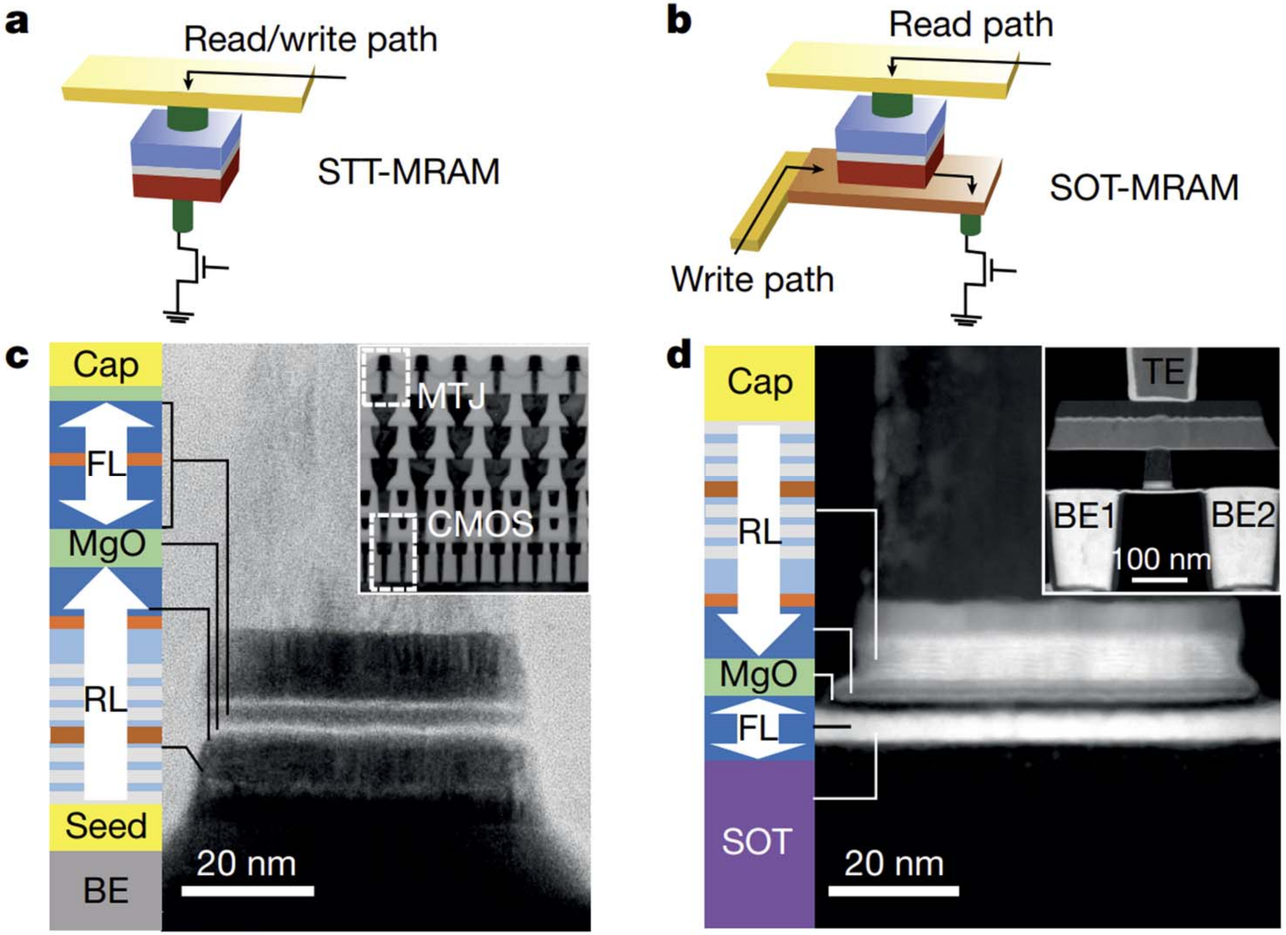
Linear-scaling quantum transport methodologies





Magnetic Random Access Memories (MRAMs)

Why to use spin-orbit coupling?



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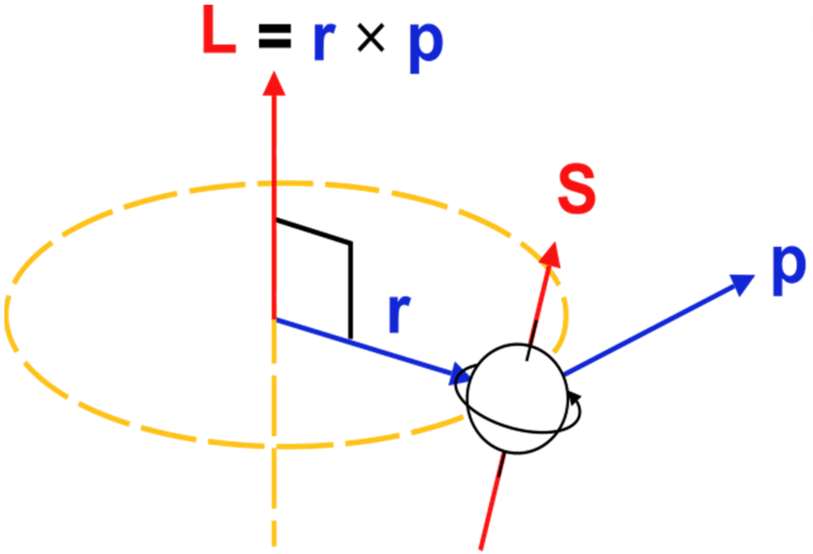
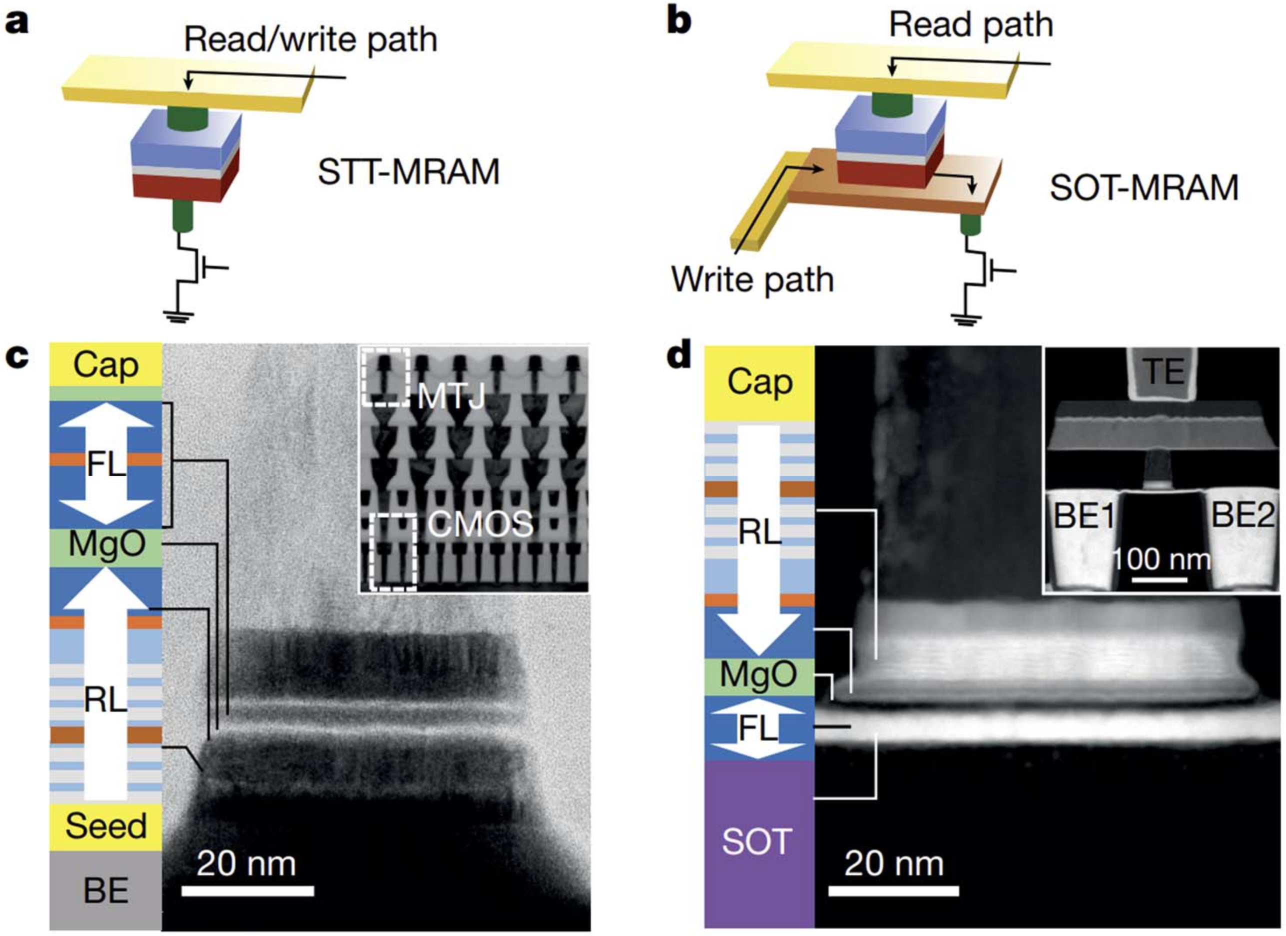
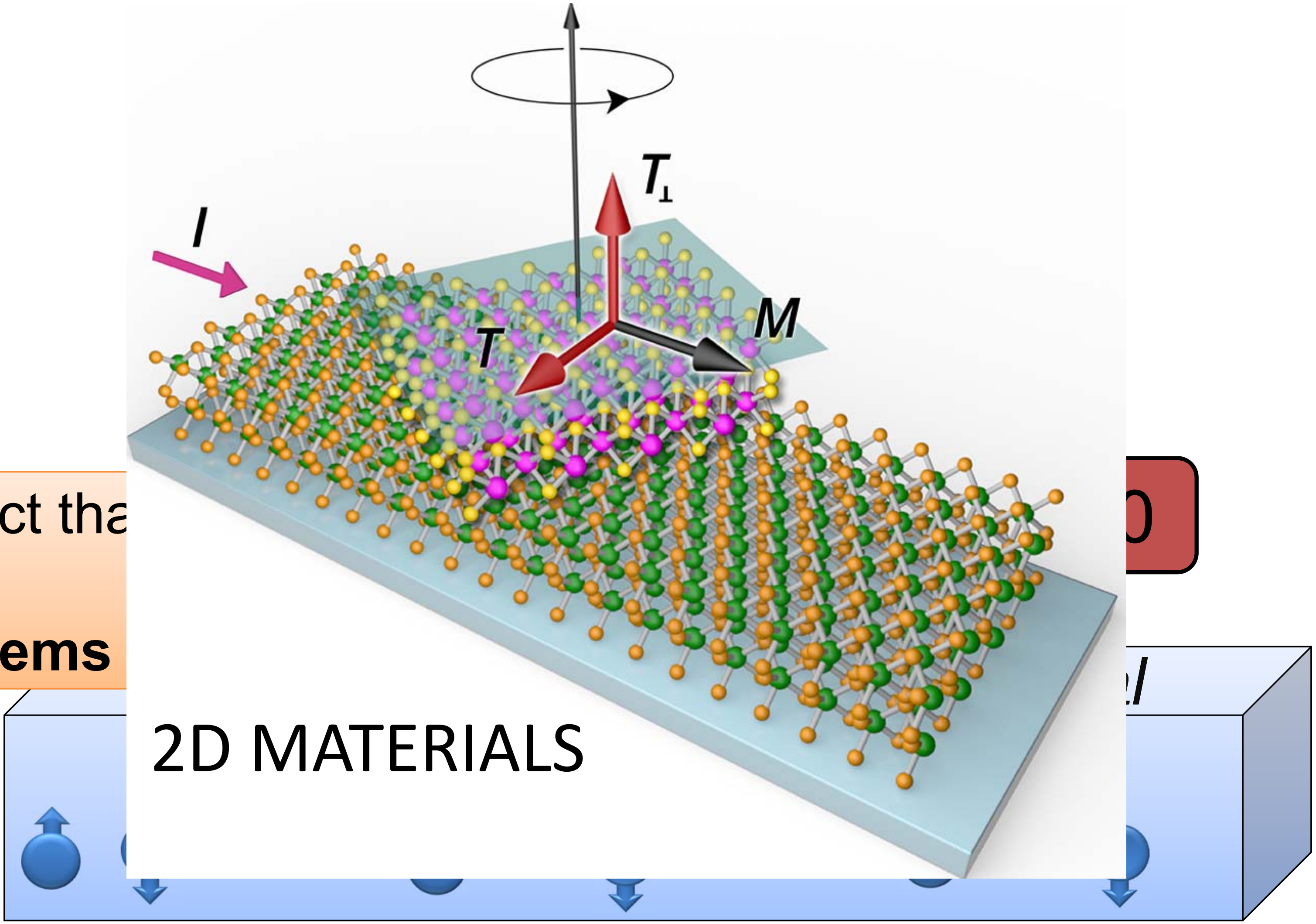




H Yang, et al, Nature **606**, pages663–673 (2022)

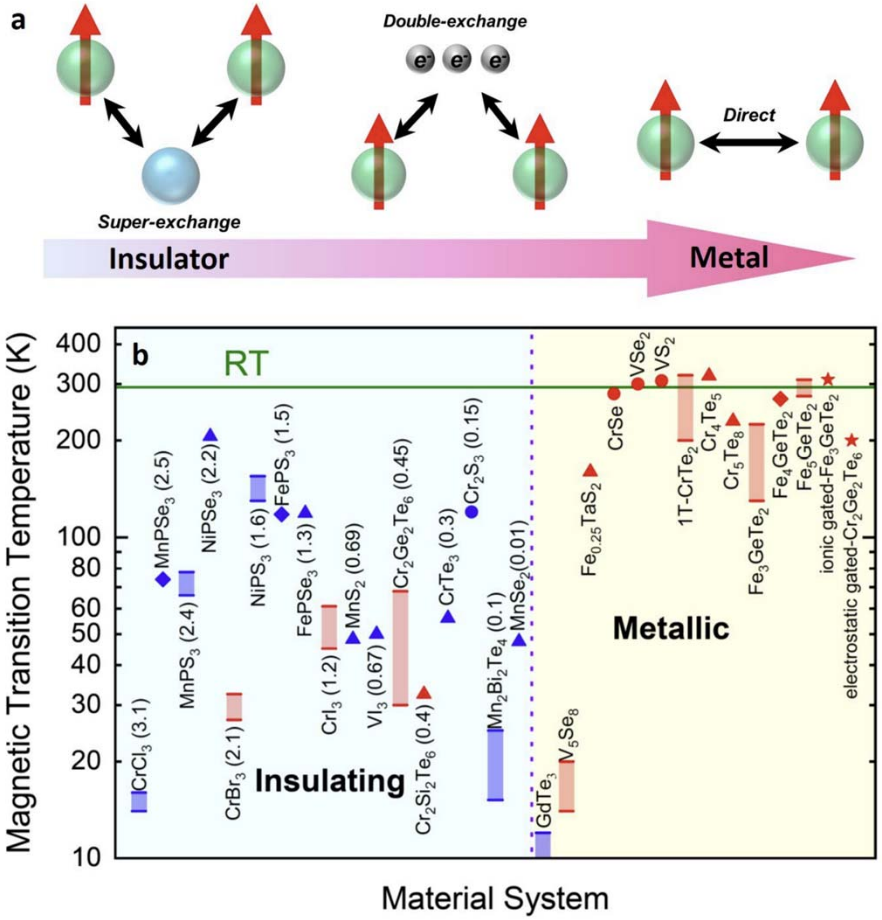
HOW DOES SOT MRAM WORK?

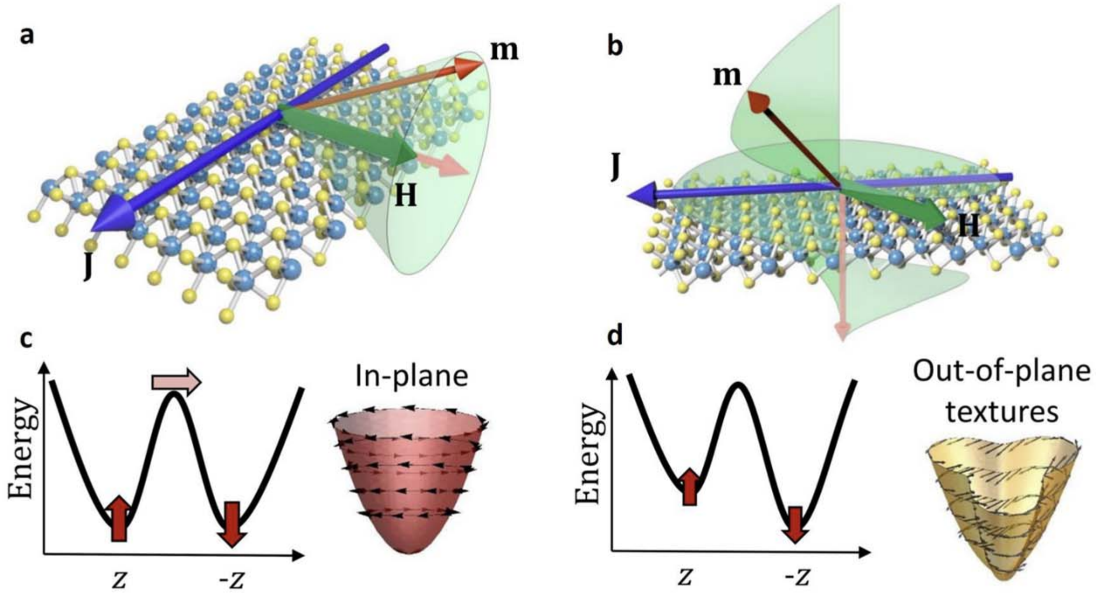
Interfacial effect tha
constrains to
ultrathin systems



2D MATERIALS

Two-dimensional magnets





H Kurebayashi, Jose H. Garcia, Safe Khan, Jairo Sinova & Stephan Roche
Nature Reviews Physics volume 4, pages150–166 (2022)

Linear-scaling quantum transport methodologies

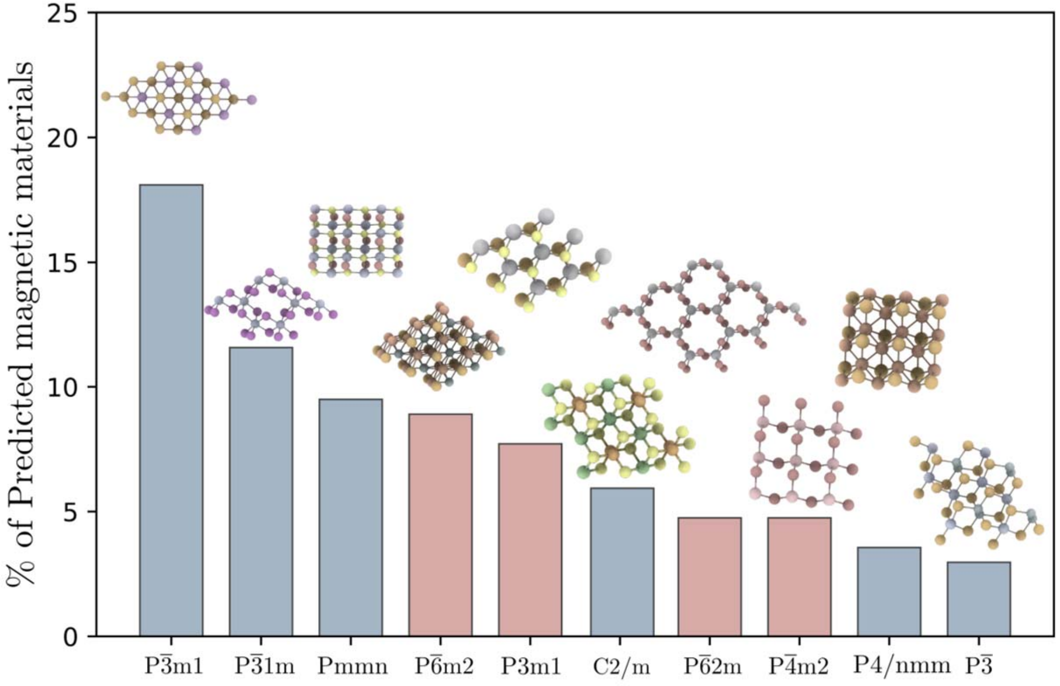


Table 1

Repr. Mat.	Space Group	Crystal System	$\mathbf{H^e}$	$\mathbf{H^o}$
$MX_3{}^*$	$P\bar{6}2m$ (189)	Hexagonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\boldsymbol{\nabla}_{\mathbf{m}}[\,J_y\,m_x m_y+J_x(m_y^2-m_x^2)/2]$
$Fe_3GeTe_2{}^*$	$P\bar{6}m2$ (187)			$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\boldsymbol{\nabla}_{\mathbf{m}}[\,J_x\,m_x m_y+J_y(m_x^2-m_y^2)/2]$
$MnBi_2Te_2$	$P\bar{3}m1$ (164)	Trigonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\boldsymbol{\nabla}_{\mathbf{m}}[\,J_x\,m_x m_y+J_y(m_x^2-m_y^2)/2]$
$MXY^{\dagger}$	P3m1 (156)			
Fe_5GeTe_2	$R\bar{3}m$ (147)			
CrI_3	$P\bar{3}1m$ (162)			$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\boldsymbol{\nabla}_{\mathbf{m}}[\,J_y\,m_x m_y+J_x(m_y^2-m_x^2)/2]$
$CrGeTe_3$	$P\bar{3}$ (147)	Trigonal	$\tau_{FL}^{I}\,\mathbf{J}\times\hat{\mathbf{z}}+\tau_F^{II}\,\mathbf{J}$	$\tau_{DL}^{I}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}^{I}\boldsymbol{\nabla}_{\mathbf{m}}\left[J_y\,m_x m_y+\frac{J_x(m_x^2-m_y^2)}{2}\right]+\tau_{ani}^{II}\boldsymbol{\nabla}_{\mathbf{m}}\left[J_y\,m_x m_y+\frac{J_x(m_x^2-m_y^2)}{2}\right]+\tau_o^{II}[(\mathbf{J}\times\boldsymbol{m})\cdot\hat{\mathbf{z}}]\hat{\mathbf{z}}$
$FeTe^{\dagger}$	P4/nmm (129)	Tetragonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	$\tau_o\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}$
CrI_2	$P\bar{4}m2$ (115)	Orthorhombic	$\begin{pmatrix}0 & \tau_{FL}^{xy}\\ \tau_{FL}^{yx} & 0\end{pmatrix}\mathbf{J}$	$(\mathbf{M}\cdot\hat{\mathbf{z}})\begin{pmatrix}\tau_z^x & 0\\ 0 & \tau_z^y\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^x & 0\\ 0 & \tau_o^y\end{pmatrix}\mathbf{J}\;\hat{\mathbf{z}}$
CrSBr	Pnmm (59)	Orthorhombic	$\begin{pmatrix}0 & \tau_{FL}^{xy}\\ \tau_{FL}^{yx} & 0\end{pmatrix}\mathbf{J}$	$(\mathbf{M}\cdot\hat{\mathbf{z}})\begin{pmatrix}\tau_z^x & 0\\ 0 & \tau_z^y\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^x & 0\\ 0 & \tau_o^y\end{pmatrix}\mathbf{J}\;\hat{\mathbf{z}}$
$NiPS_3$	C2/m (12)	Monoclinic	$\begin{pmatrix}0 & \tau_{FL}^{xy} & 0\\ \tau_{FL}^{yx} & 0 & 0\\ 0 & \tau_{FL}^{yz} & 0\end{pmatrix}\mathbf{J}$	$\begin{pmatrix}M_x\,\tau_o^{x,xx}+M_z\,\tau_o^{z,xx} & M_y\,\tau_o^{y,yx} & 0\\ M_y\,\tau_o^{y,xy} & M_x\,\tau_o^{x,yy}+M_z\,\tau_o^{z,yy} & 0\\ M_z\,\tau_o^{z,xz} & 0 & 0\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^{xx} & 0 & 0\\ 0 & \tau_o^{yy} & 0\\ 0 & 0 & 0\end{pmatrix}\mathbf{J}\,\hat{\mathbf{z}}$

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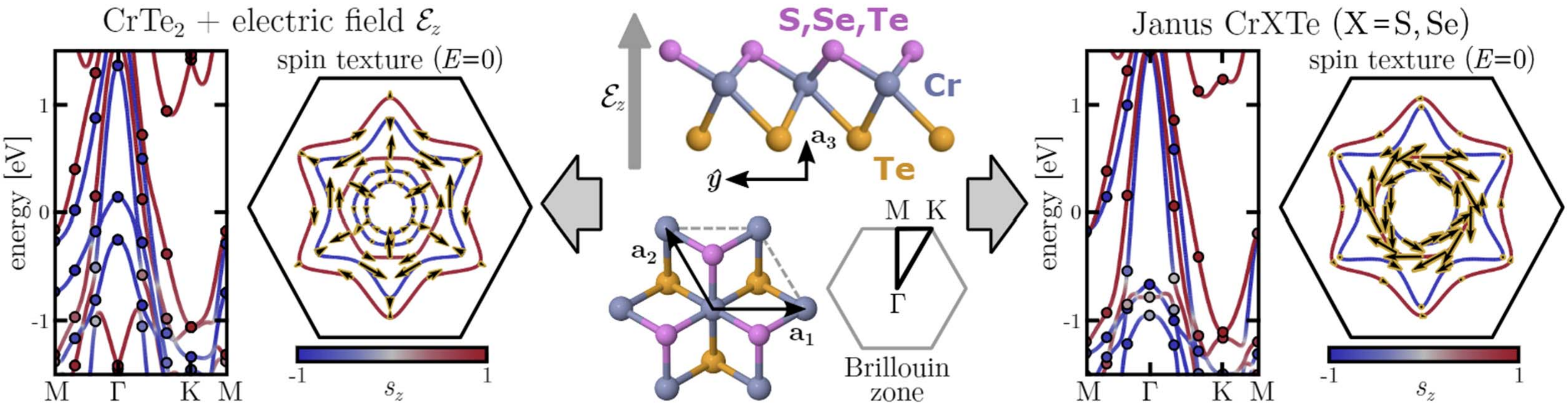
Janus Cr-based Family as a platform for SOT-MRAM



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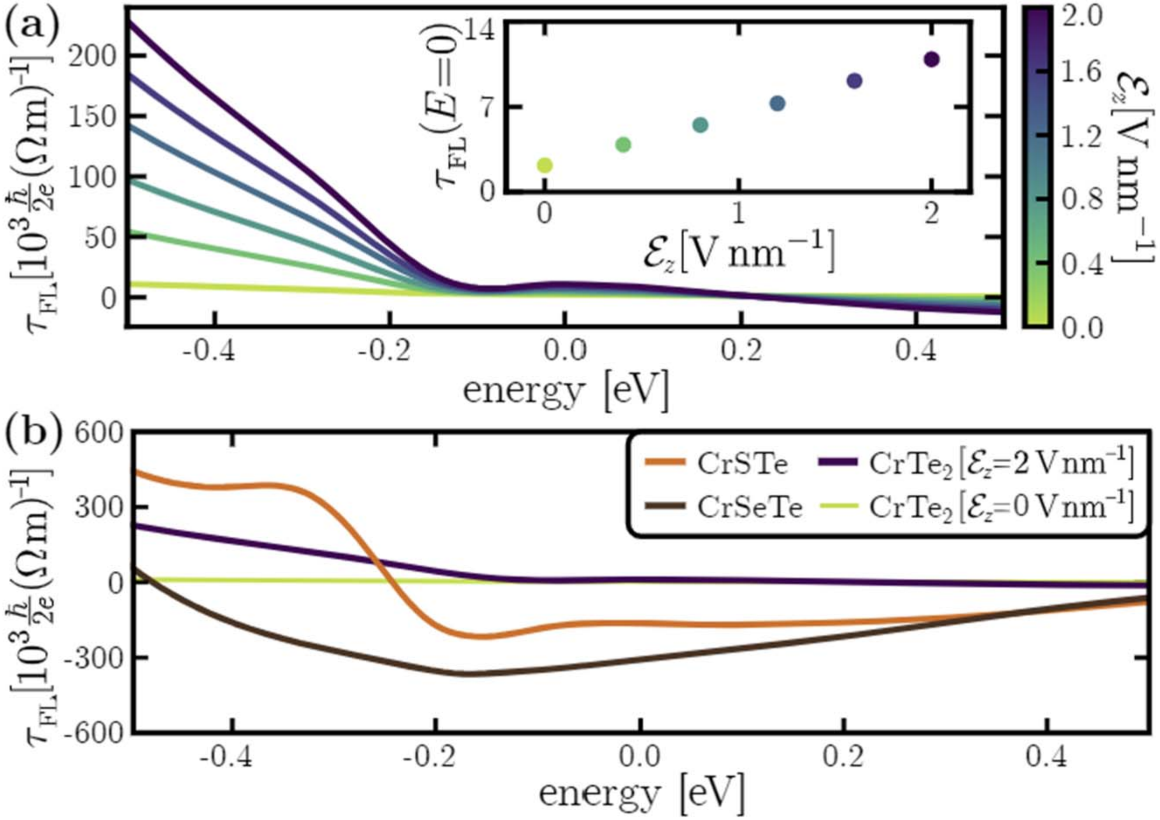

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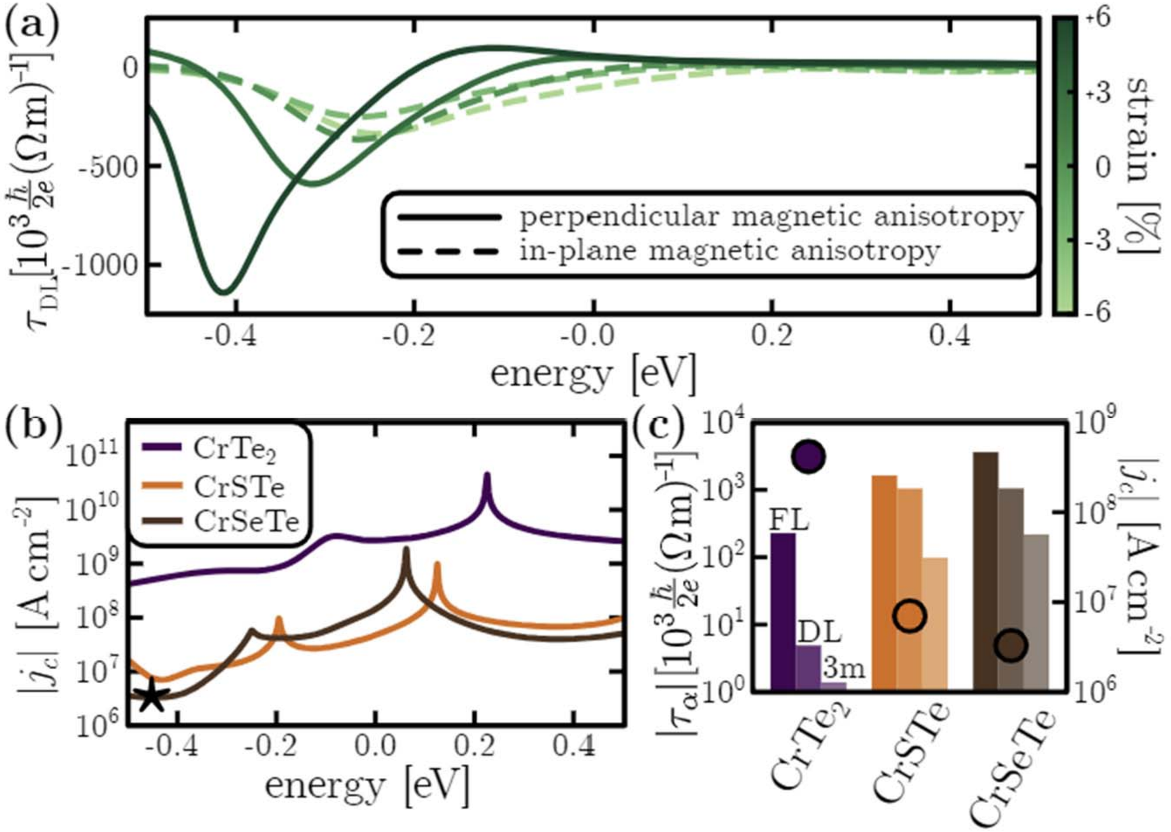

- Two-dimensional materials are showing great promise for highly optimized non-volatile magnetic random access memories (MRAM), thanks to their interfacial characteristics, high tunability, and compatibility with existing technologies. Currently, Cr-based magnetic Janus materials appear to be among the most promising candidates, offering critical switching currents on par with those of the leading metal/magnetic interfaces.

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THANK YOU

ICOS
International Cooperation
On Semiconductors

European
Commission

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