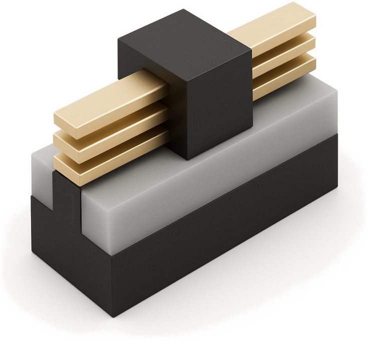
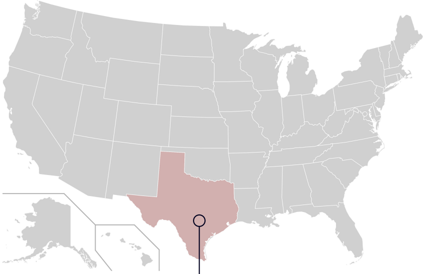
High-throughput computing, cloud cyberinfrastructure, and machine learning for semiconductor design

Feliciano Giustino

Oden Institute & Department of Physics

University of Texas at Austin





University of Texas at Austin

ODEN INSTITUTE FOR COMPUTATIONAL ENGINEERING & SCIENCES

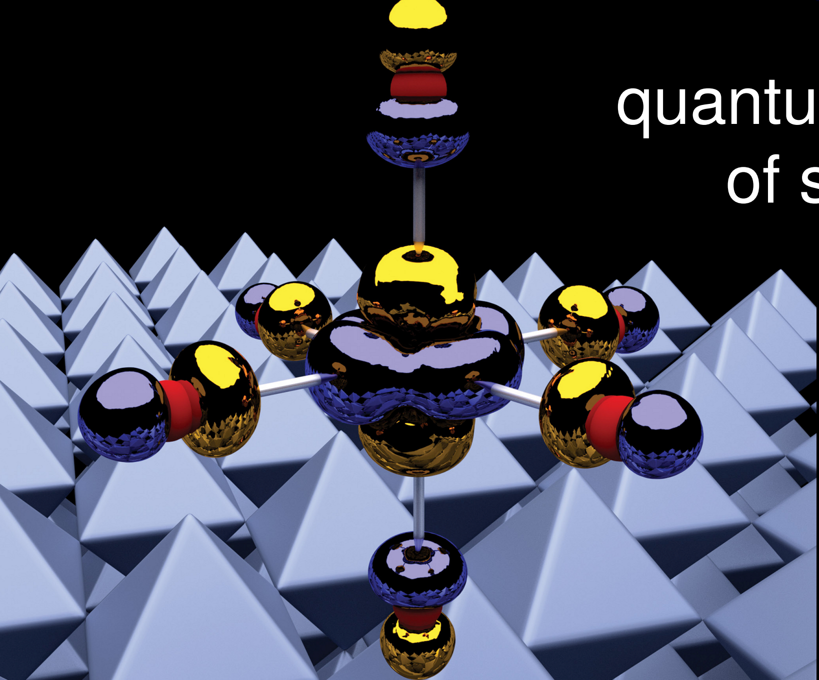
TACC

NSF

NSF LEADERSHIP-CLASS COMPUTING FACILITY
TEXAS ADVANCED COMPUTING CENTER
THE UNIVERSITY OF TEXAS AT AUSTIN

A research community where computing, mathematics, science and engineering come together to conduct interdisciplinary research and education

quantum theory of solids




high-performance
computing
eliashberg_aniso_cont_raxis.f90
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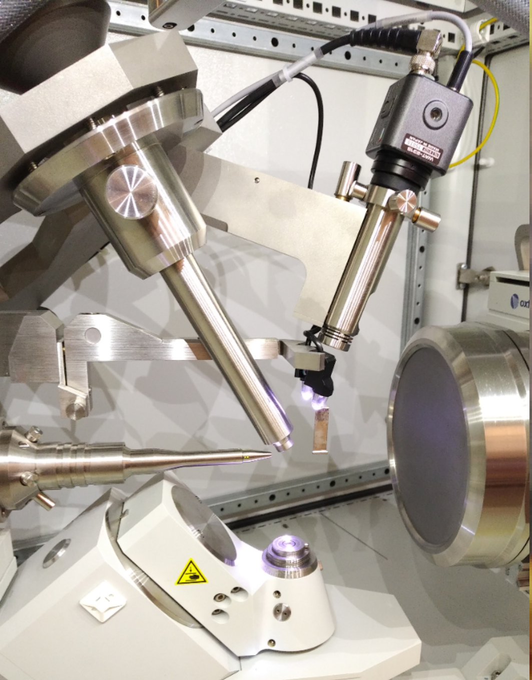
eliashberg_pp.f90
eliashberg_readfiles.f90
eliashberg_setup.f90
eliashberg_write.f90
eliashberg.f90
eliashbergcom.f90
elph2.f90
elphel2_shuffle.f90
elphon_shuffle_wrap.f90
elphon_shuffle.f90
ephbloch2wane.f90
ephbloch2wanp.f90
ephwan2bloch_mem.f90
ephwan2bloch.f90
ephwan2blochp_mem.f90
ephwan2blochp.f90 3
ephwann_shuffle_mem.f90
ephwann_shuffle.f90
epw_init.f90
epw_readin.f90
epw_setup.f90
epw_summary.f90
epw.f90 1
epw.x
epwcom.f90
fermiwindow.f90
gen_freqgrid.f90
gmap_sym.f90
hambloch2wan.f90
hamwan2bloch.f90
io_dyn_mat2.f90
io_epw.f90
OUTLINE
#if defined(__MPI)
INTEGER (kind=MPI_OFFSET_KIND) :: lrepmatw
!! Offset to tell where to start reading the fil
INTEGER (kind=MPI_OFFSET_KIND) :: lrepmatw2
!! Offset to tell where to start reading the
#else
INTEGER(kind=8) :: lrepmatw
!! Offset to tell where to start rea
INTEGER(kind=8) :: lrepmatw2
!! Offset to tell where to start
#endif
!
REAL(kind=DP) :: rdotk
!! Exponential for the
!
COMPLEX(kind=DP)
!! Temporary mat
COMPLEX(kind=DP)
!! Factor for the
COMPLEX(kind=DP)
!! El-ph matrix e
!
CALL start_clock('e
!--------------------
! STEP 3: inverse Fou
!---------------------
!
! g~ (k') = sum_R 1/ndege
!
! g~(k') is epmatf (nmodes,
! every pool works with its
!
IF (parallel_k) THEN
CALL para_bounds(ir_start, ir_
ELSEIF (parallel_q) THEN
ir_start = 1



computational materials discovery

Yesterday

Neural network potentials
for phonons

Jaesuk Park

Symbolic regression
for electrons

Nick Pant

Today

2D Materials

Viet-Anh Ha

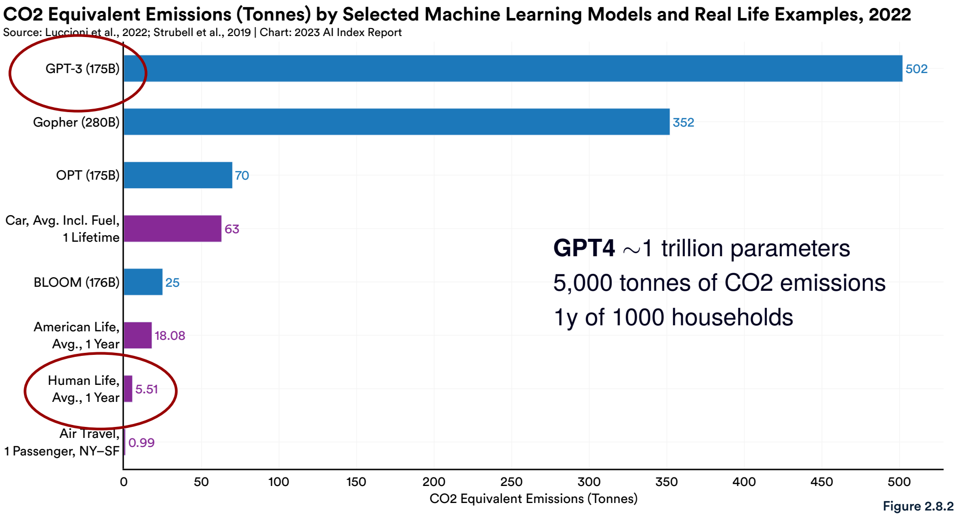
GPU acceleration

Tae Yun Kim

EPWpy and CSSI

Sabyasachi Tiwari

How much energy does it take to train LLMs



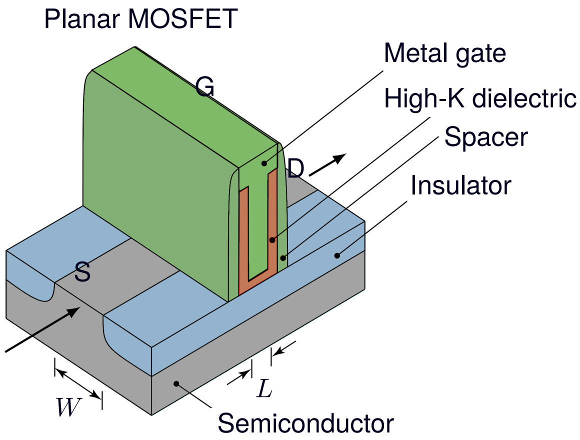
GPT4 ~1 trillion parameters

5,000 tonnes of CO_2 emissions

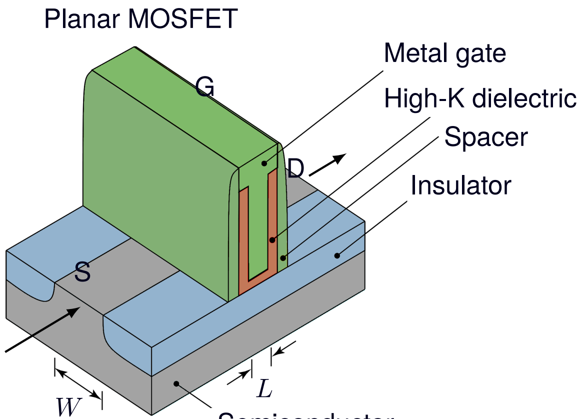
1y of 1000 households

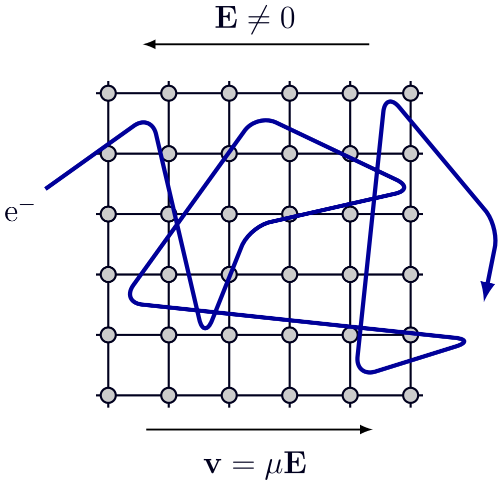
Figure from: Maslej et al, *The AI Index 2023 Annual Report*, Institute for Human-Centered AI, Stanford

Field effect transistor



Field effect transistor

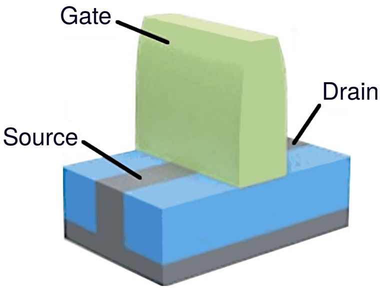




μ carrier mobility

Evolution of FET layout

Planar FET



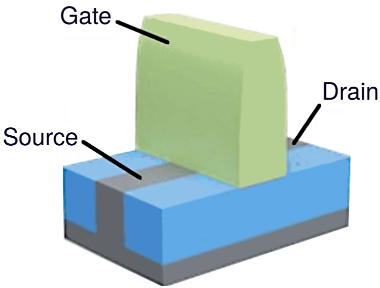
1971

Intel 4004 chip
10μm process
2,300 transistors

Figure from: Draeger, https://newsroom.lamresearch.com (2020)

Evolution of FET layout

Planar FET



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Intel 4004 chip
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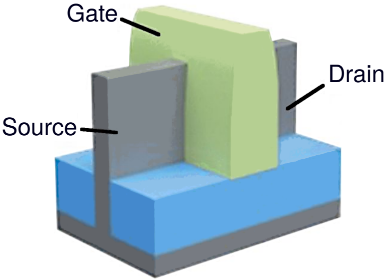
FinFET



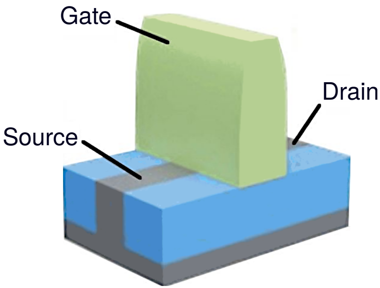
2012

Intel Ivy Bridge chip
22nm process
1.4 billion transistors

Figure from: Draeger, https://newsroom.lamresearch.com (2020)

Evolution of FET layout

Planar FET



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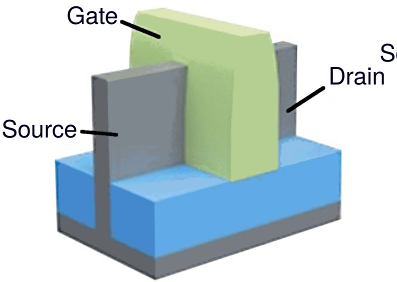
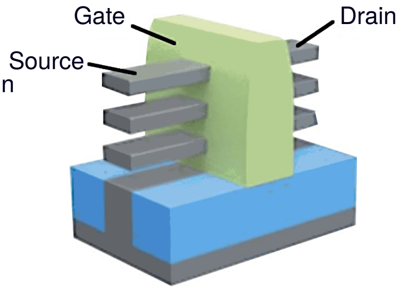
FinFET



2012

Intel Ivy Bridge chip
22nm process
1.4 billion transistors

GAAFET or RibbonFET

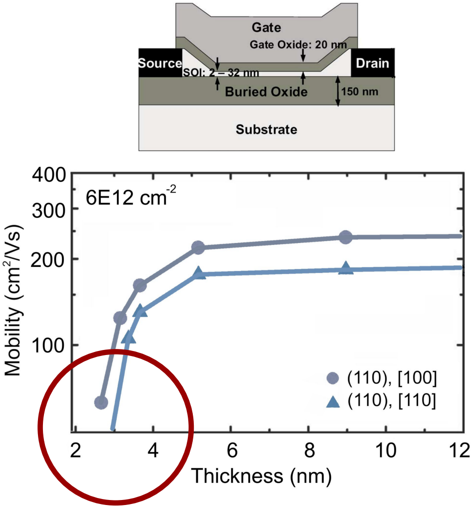


2022

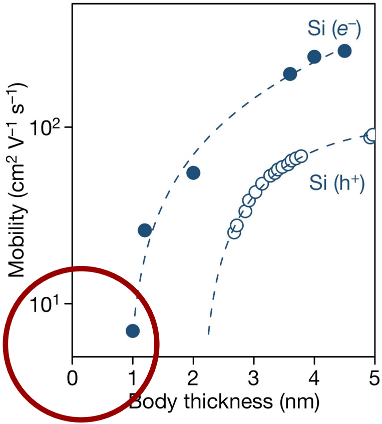
Apple A16 Bionic chip
TSMC 4nm process
16 billion transistors

Figure from: Draeger, https://newsroom.lamresearch.com (2020)

Degradation of carrier mobility in ultrathin silicon



Bulk Si mobility: 1400 cm^2/Vs



Left figures from: Tsutsui Hiramoto, IEEE Trans. Electron Devices 53, 2582 (2006)

Right figure from: Liu et al, Nature 591, 43 (2021)

The promise of 2D semiconductors

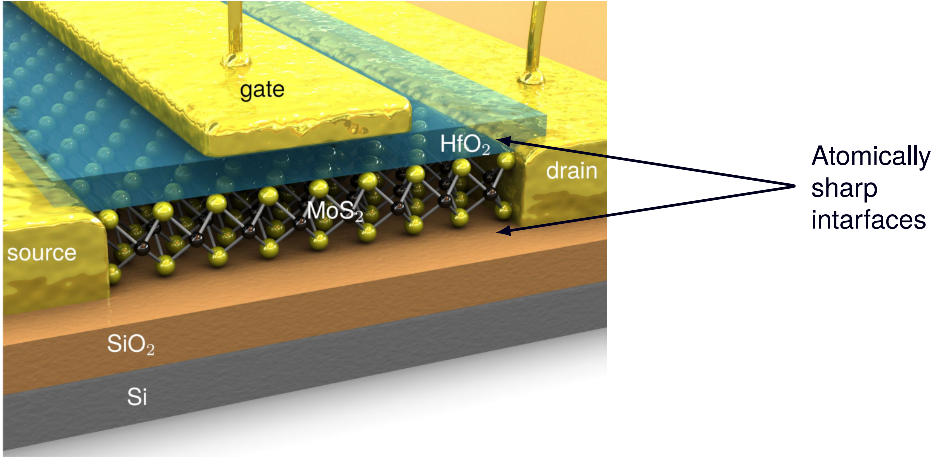
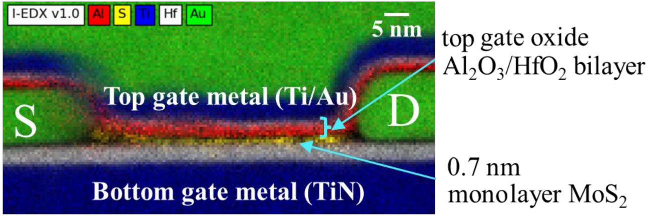
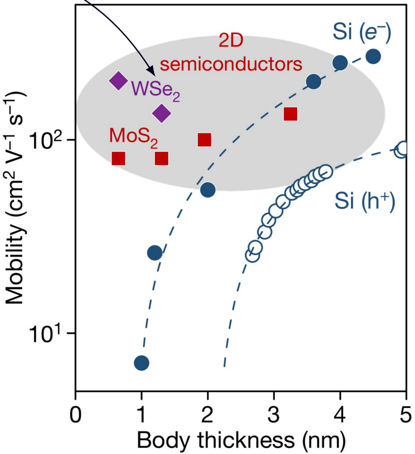


Figure from: Figure from: Radisavljevic, Kis, et al, Nat. Nanotech. 6, 147 (2011)

Current limitations of 2DFETs

mobility ∼100 cm^2/Vs

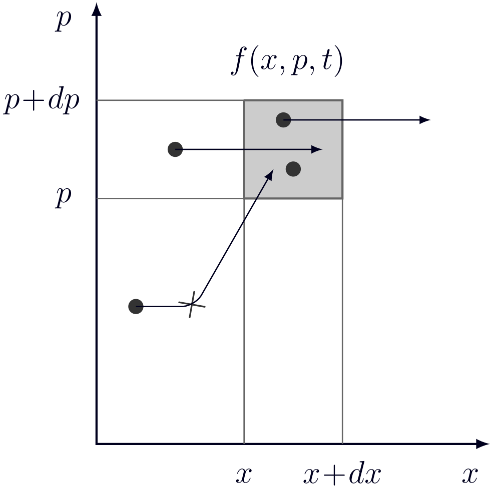




Left figure from: Dorow et al., IEDM 2022, doi: 10.1109/IEDM45625.2022.10019524

Right figure from: Liu et al, Nature 591, 43 (2021)

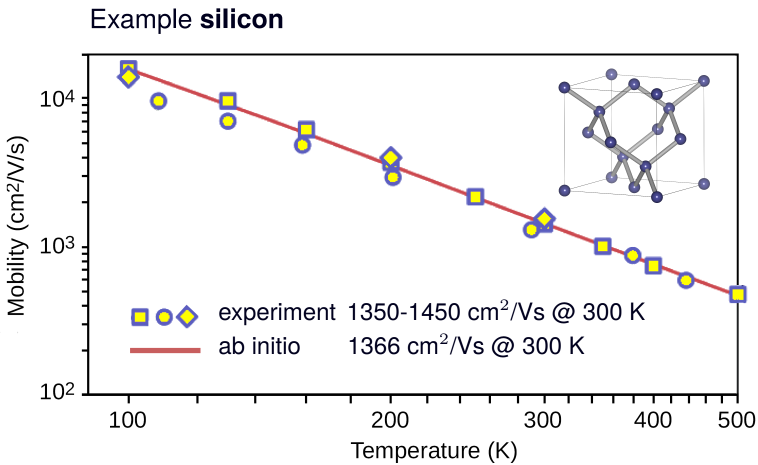
Ab initio Boltzmann transport equation



Collisionless flow — Scattering

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt} + \frac{\partial f}{\partial \mathbf{p}} \cdot \frac{d\mathbf{p}}{dt} = \Gamma_{\text{in}} - \Gamma_{\text{out}}$$

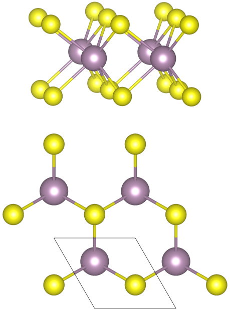
Comparison between theory and experiment

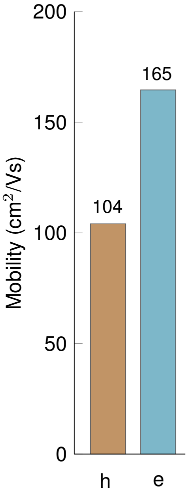


Poncé, Margine, FG, Phys. Rev. B 97, 121201 (2018)

Theory vs. experiments for 2D materials

Example **MoS_2**





Ha & FG, npj Comput. Mater. 10, 229 (2024)

Theory vs. experiments for 2D materials

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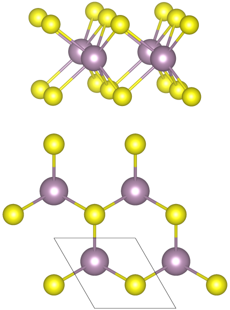
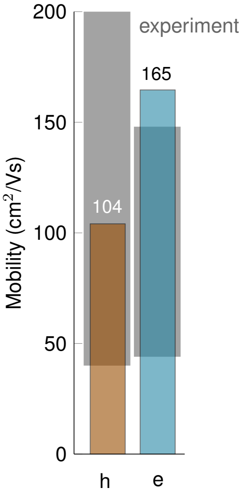


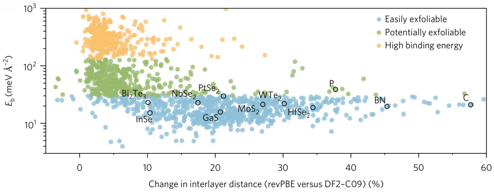


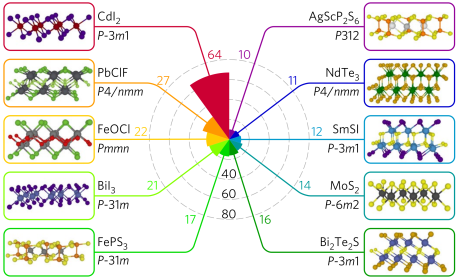
2D Materials Databases

Table 1 | Database statistics

	Unique to the ICSD	Unique to the COD	Common to both	Total sum
Experimental data				
CIF inputs	99,212	87,070		186,282
Unique 3D structures (set A)	34,548	60,354	13,521	108,423
Layered 3D structures (set B)	3,257	1,180	1,182	5,619
DFT calculations				
Layered 3D, relaxed (set C)	2,165	175	870	3,210
Binding energies (set D)	1,795	126	741	2,662
2D easily exfoliable (EE)	663	79	294	1,036
2D potentially exfoliable (PE)	524	34	231	789
Total	1,187	113	525	1,825

Experimental data: number of structures imported from the two databases (ICSD or COD, uniqueness not tested), number of unique 3D structures in each imported set or common to both (set A), and number of layered 3D structures identified using the geometrical criteria discussed in the text (set B). DFT calculations: number of structures that were relaxed (set C), number of structures that remain classified as layered after relaxation and for which binding energies were computed (set D), and number of easily or potentially (see text) exfoliable compounds.

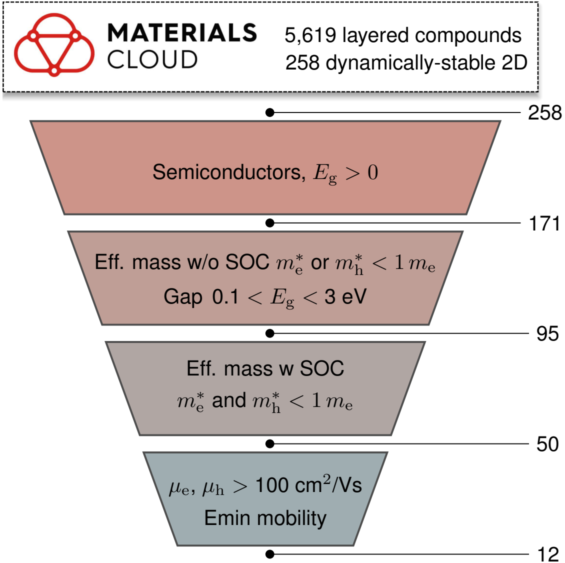




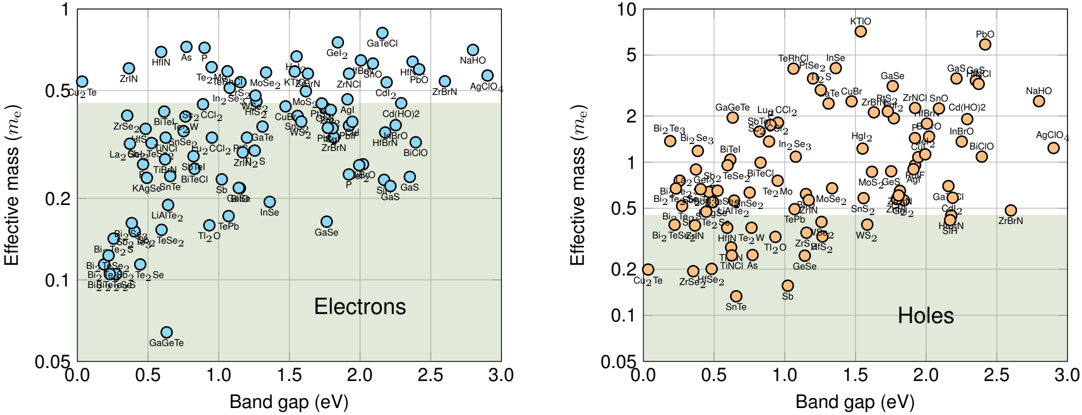
Figures from: *Materials Cloud 2D Datadase*, Mounet, Marzari, et al, Nat Nanotech 13, 246 (2018)

See also: *Computational 2D Materials Database*, Haastrup, Thygesen, et al, 2D Materials 5, 042002 (2018)

High-throughput screening workflow

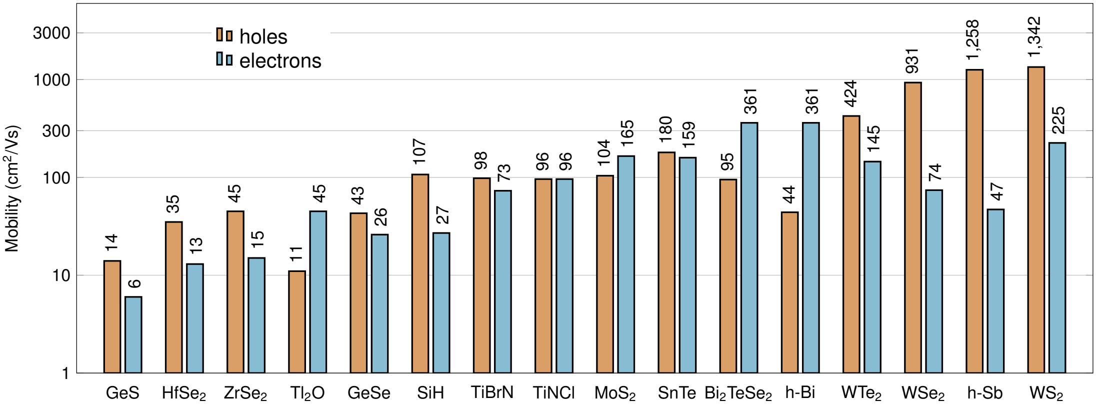


Pre-screening via effective masses



Set effective mass cutoff to 0.45 m_e based on 100 cm^2/Vs mobility target

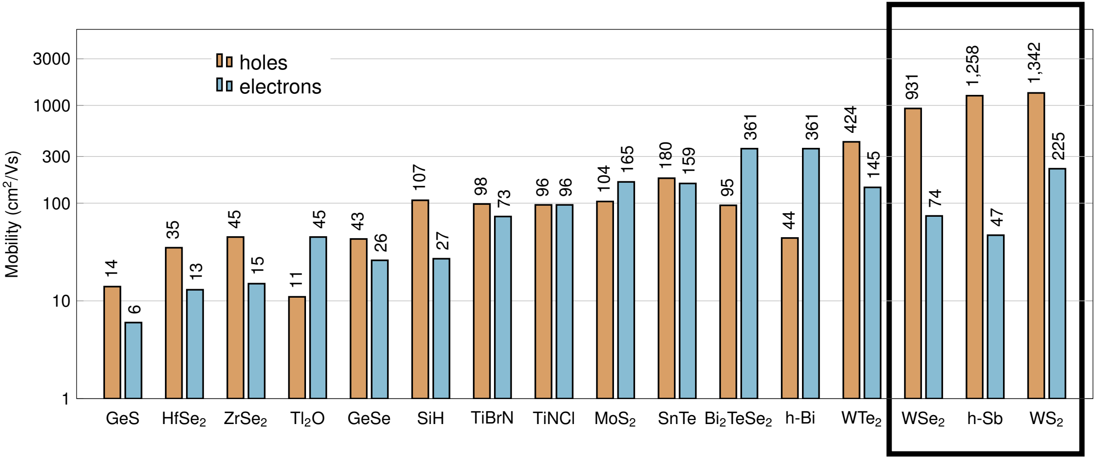
Top 2D semiconductors from *ab initio* BTE



Ha & FG, npj Comput. Mater. 10, 229 (2024)

See also: Cheng et al, JACS 140, 17895 (2018); JACS 141, 16296 (2019); PRL 125, 177701 (2020)

Top 2D semiconductors from *ab initio* BTE



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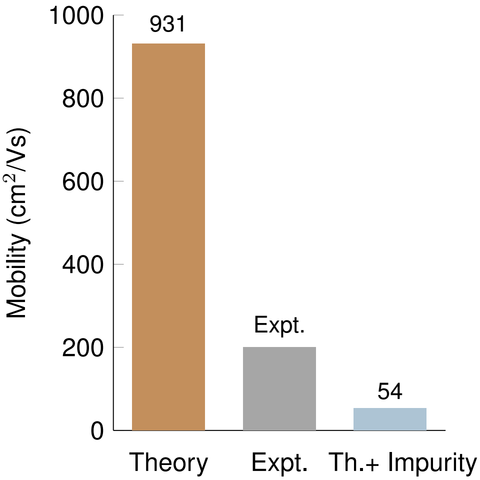
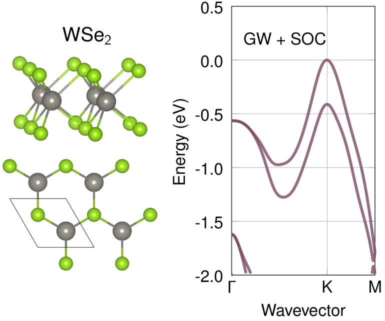
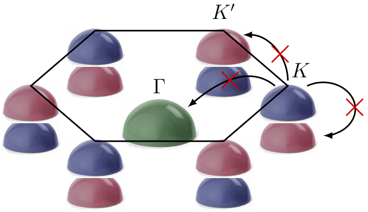
See also: Cheng et al, JACS 140, 17895 (2018); JACS 141, 16296 (2019); PRL 125, 177701 (2020)

Spin-valley locking in WSe_2 boosts mobility

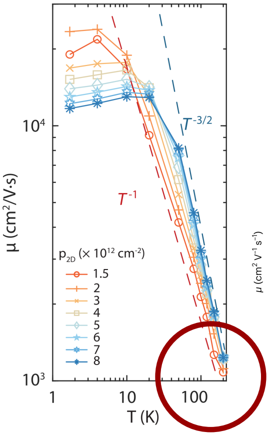


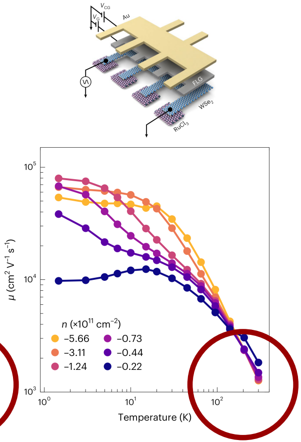




Ha & FG, npj Comput. Mater. 10, 229 (2024)

Recent measurements of high-quality WSe_2 samples

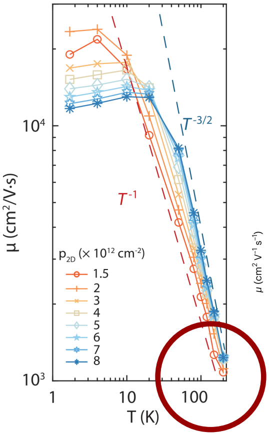


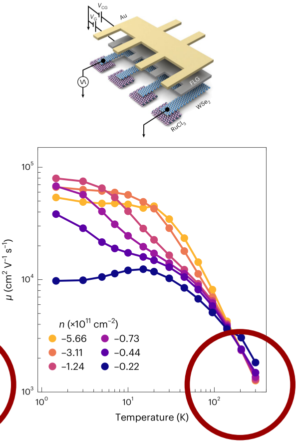


Left figures from: Joe, Kim, et al, Phys. Rev. Lett. 132, 056303 (2024)

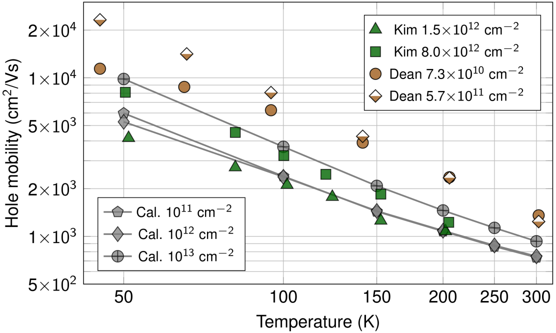
Middle figures from: Pack, Dean, et al, Nat. Nanotechnol. 19, 948 (2024)

Recent measurements of high-quality WSe_2 samples





Successfully **predicted** by *ai*BTE



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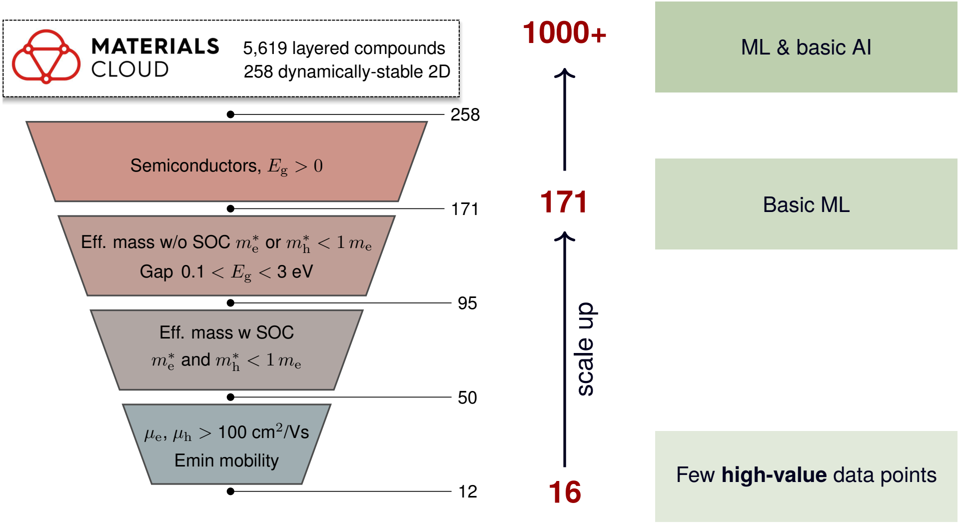
High-throughput screening workflow



The EPW software project

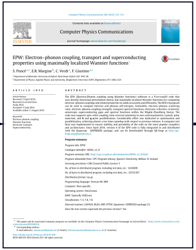

PHYSICAL REVIEW B 76, 165108 (2007)

Electron-phonon interaction using Wannier functions

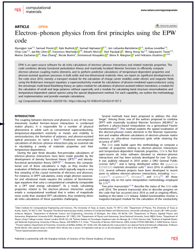
Feliciano Giustino, Marvin L. Cohen, and Steven G. Louie


Computer Physics Communications

EPW: A program for calculating the electron–phonon coupling using maximally localized Wannier functions


Computer Physics Communications

EPW: Electron–phonon coupling, transport and superconducting properties using maximally localized Wannier functions


npj computational materials

Electron–phonon physics from first principles using the EPW code

2007	2010	2016	2025
v2.1.5 1,733 LOC	v2.3.5 16,889 LOC	v4.1 30,681 LOC	v6.0 104,251 LOC

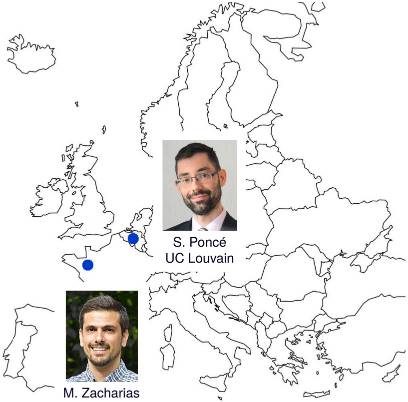
The EPW Collaboration

E. Kioupakis
U Michigan

R. Margine
U Binghamton

S. Tiwari
UT Austin

F. Giustino
UT Austin



S. Poncé
UC Louvain

M. Zacharias
U Rennes

F. Caruso
U Kiel

Y.-W. Son
KIAS

Current developers

Kyle Bushick
Fabio Caruso
Jie-Cheng Chen
Zhenbang Dai
Feliciano Giustino
Viet-Anh Ha
Emmanouil Kioupakis
Jon Lafuente-Bartolomé
Tae Yun Kim
Chao Lian
Jae-Mo Lihm
Zhe Liu
Roxana Margine
Hitoshi Mori
Yiming Pan
Samuel Poncé
Danylo Radevych
Young-Woo Son
Sabyasachi Tiwari
Aidan Thorn
Shashi Mishra
Amanda Wang
Wooil Yang
Marios Zacharias
Xiao Zhang

Hybrid MPI/OpenMP in EPW and full-system runs on Frontera

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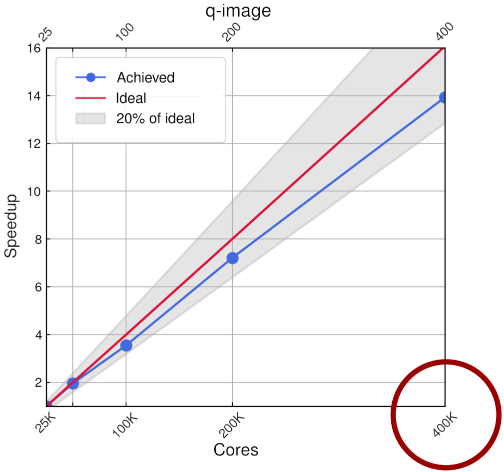
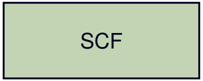
Electron **scattering rates** of MoS_2



Implementation and scaling tests by S. Tiwari, UT Austin (2025)

Taming the complexity of advanced calculations



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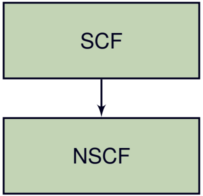

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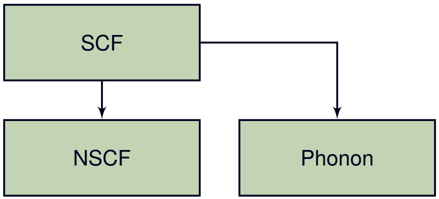

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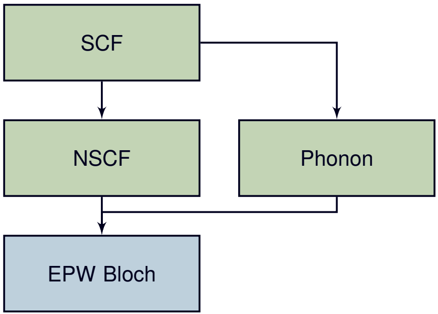

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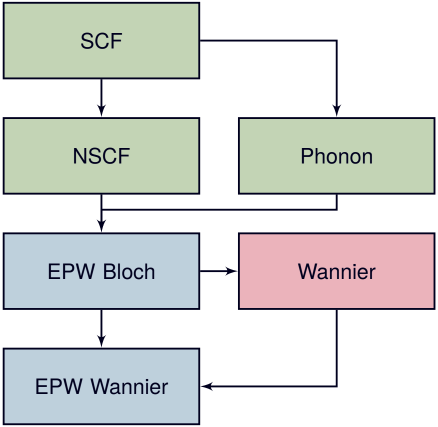
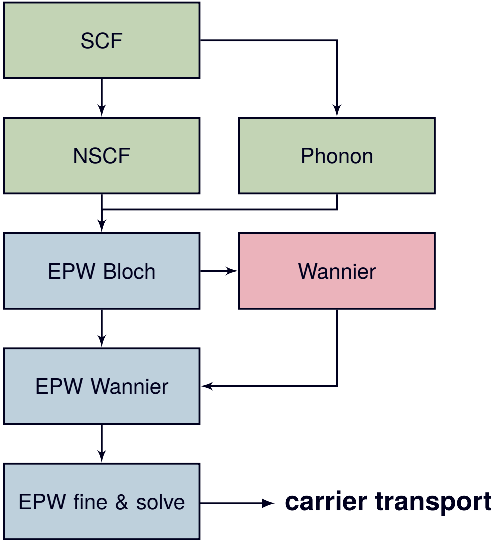
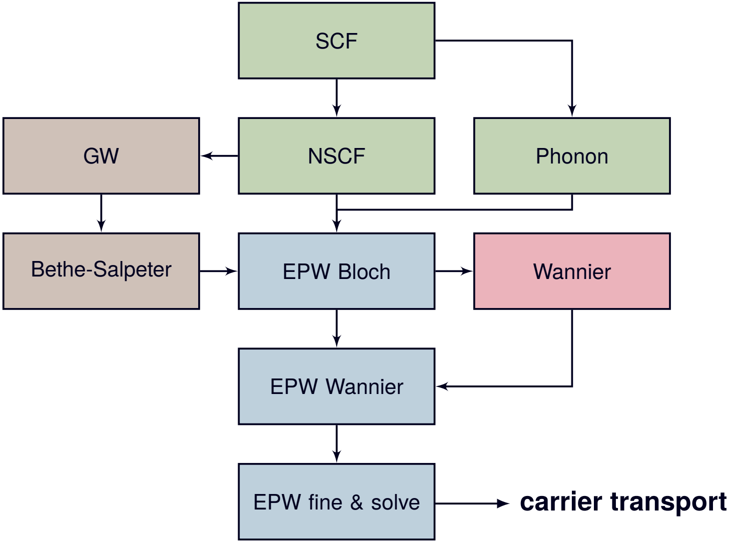


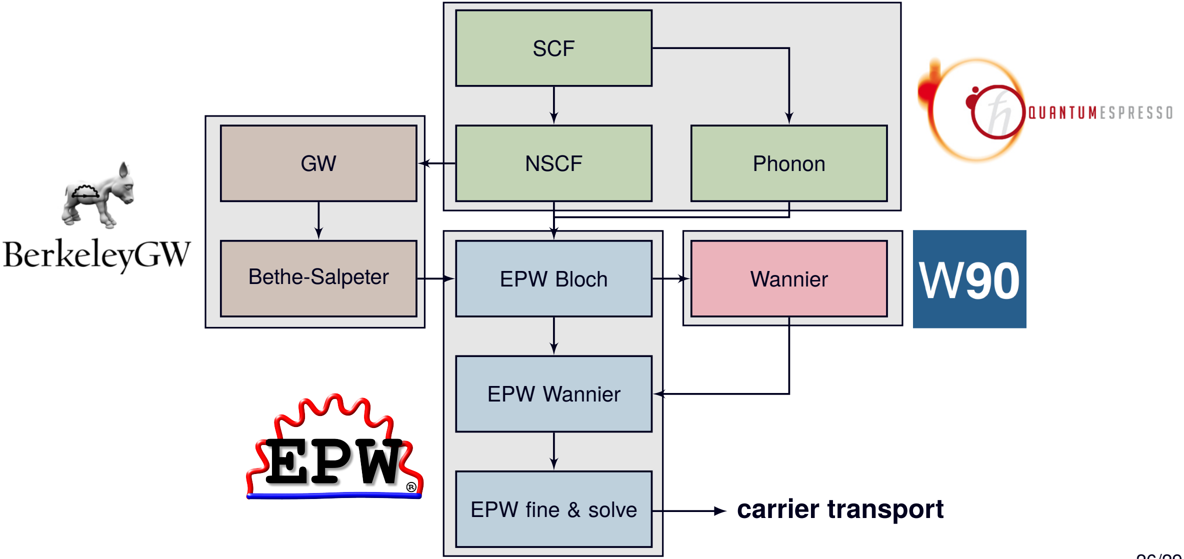
Taming the complexity of advanced calculations



Taming the complexity of advanced calculations



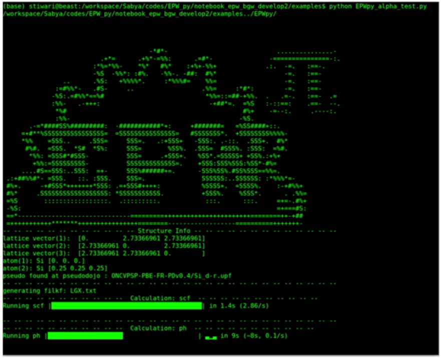
Taming the complexity of advanced calculations



Abstraction, automation, and interoperability with EPWpy

https://epwpy.org

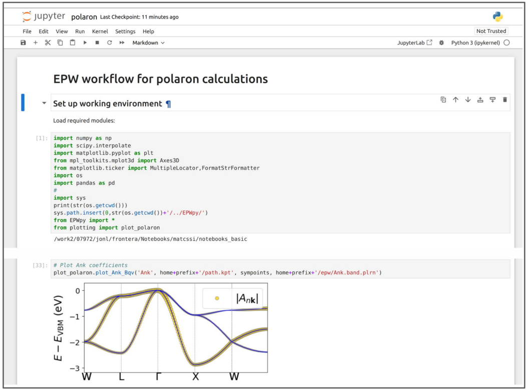
```python
silicon = EPWpy({'MatProjID':'mp-149','pseudo_auto':True},code=QE)
silicon.scf(kpoints={'kpoints':[8,8,8]})
```



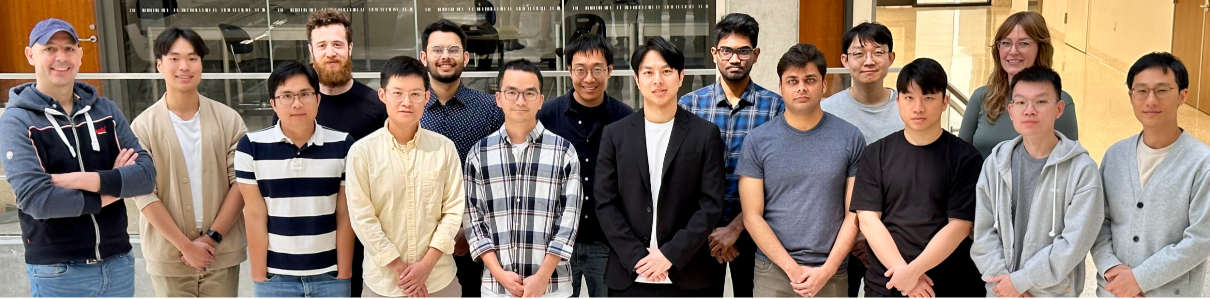
- Materials are **objects**, properties are **functions**
- Interfaces with
  - Quantum ESPRESSO
  - VASP
  - Abinit
  - BerkeleyGW
  - EPW
- Lightweight
- Intuitive for users and developers

Advanced workflows on the cloud

https://matcssi.tacc.utexas.edu



A cloud-based portal for intuitive materials modeling using **JupyterHub HPC**



UT Austin
Viet-Anh Ha
Sabyasachi Tiwari
Tae Yun Kim
Nick Pant
Jie-Cheng Chen
Abu Zubair

Cornell
Grace Xing
Debdeep Jena
Darrell Schlom

USC
Zhenglu Li

KIAS Seoul
Wooil Yang
Young-Woo Son

UC Berkeley
Steven Louie

UCSB
Chris Van de Walle

U Kiel
Yiming Pan
Fabio Caruso

EPW Collaboration
Roxana Margine
Samuel Poncé
Emmanouil Kioupakis
Marios Zacharias
Jon Lafuente-Bartolomé
Chao Lian

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