DRIVING THE EXASCALE TRANSITION

Materials discovery at the intersection of high-throughput and high-performance computing

Nicola Marzari, EPFL

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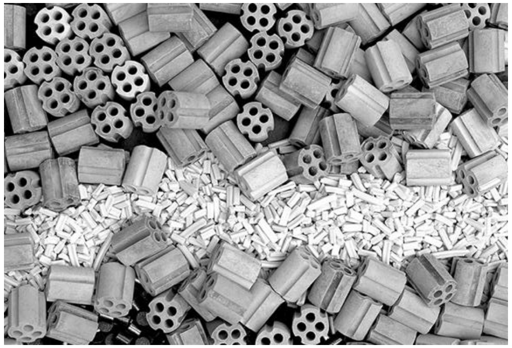
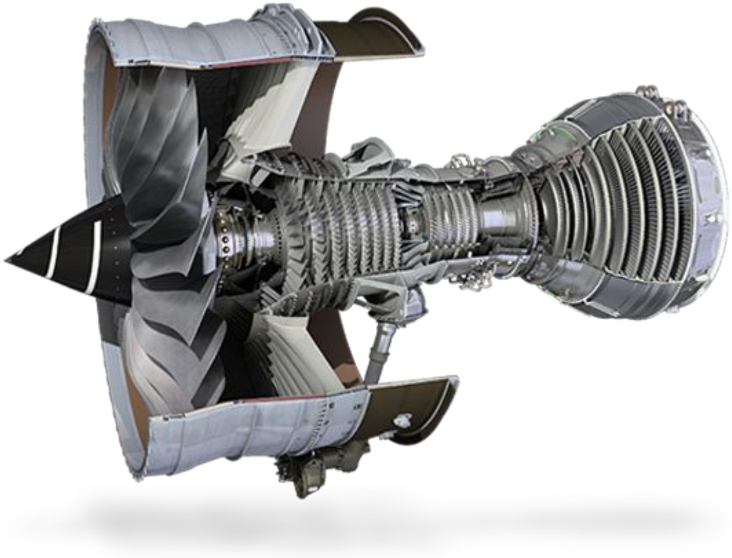
Materials enable the technologies that power our economy





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Materials enable the technologies that power our economy

- **Energy harvesting, conversion, storage, efficiency:** photovoltaics, photocatalysis, batteries, thermoelectrics, superconductors
- **Environmental protection and reparation:** CO_2 reduction, membranes for gas separation
- **Information and communication technologies:** qubits, memristors, low-dim FET, optoelectronic handshaking, storage
- **High-tech/high-value industries:** additive manufacturing
- **Pharma:** crystallization and stability

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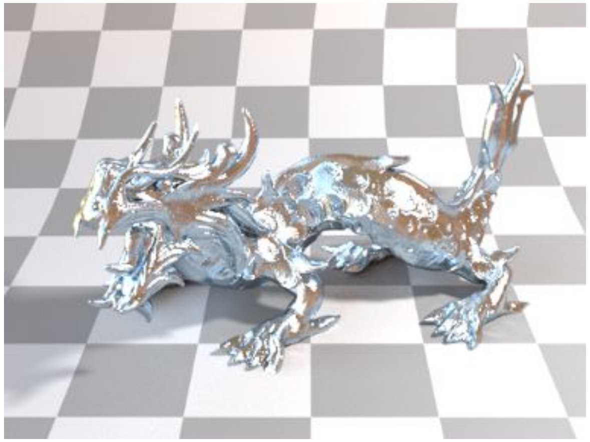
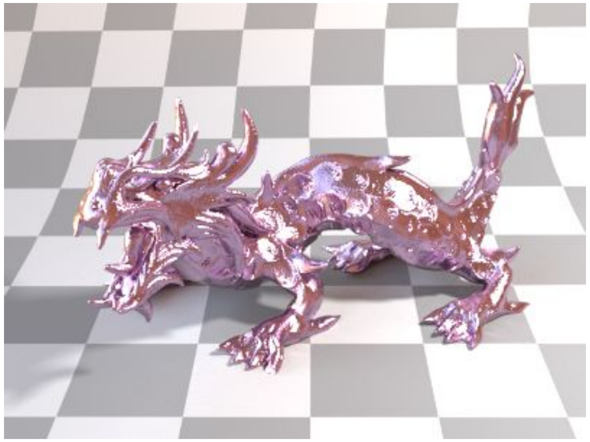
First-principles predictions of materials properties





G. Prandini, G.M. Rignanese, and N. Marzari, npj Computational Materials 5, 129 (2019)

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First-principles predictions of materials properties

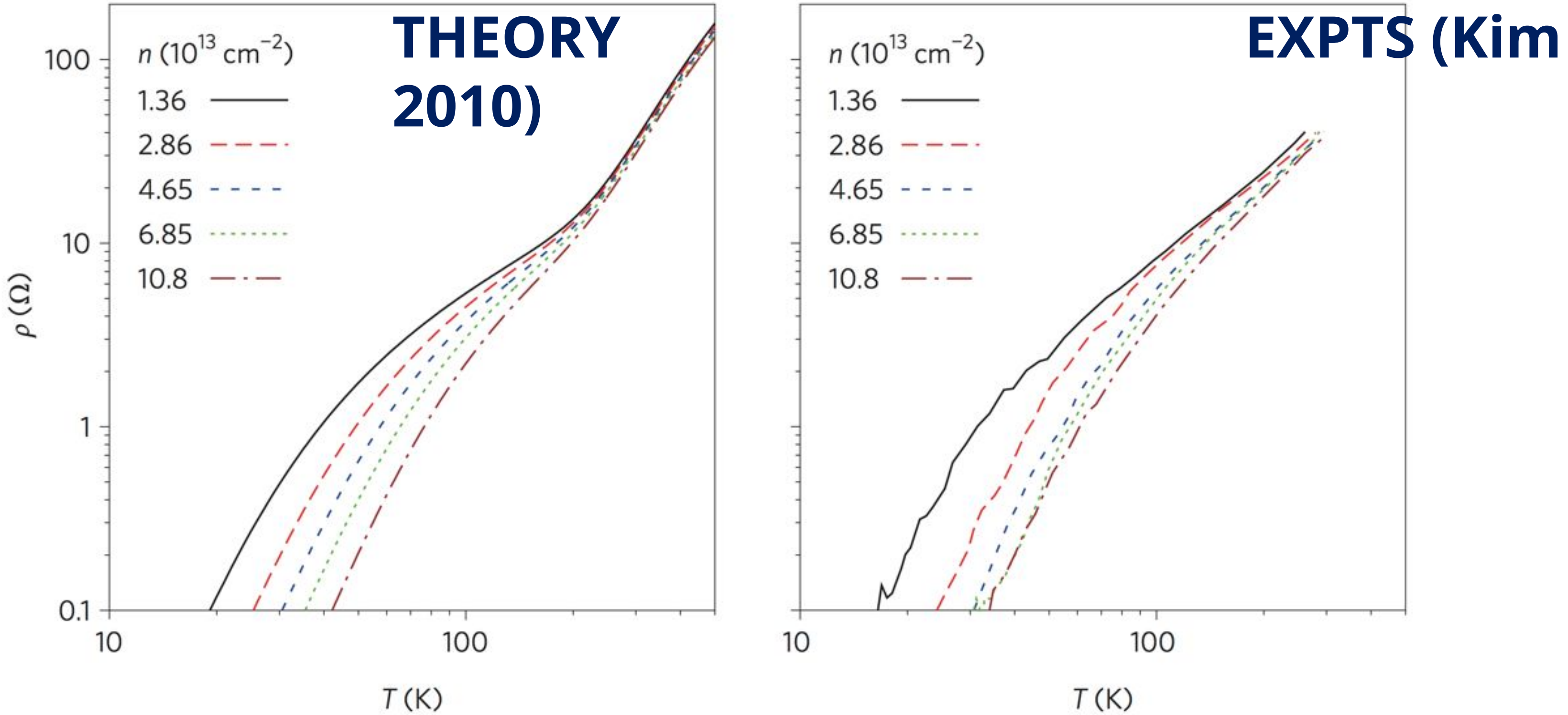


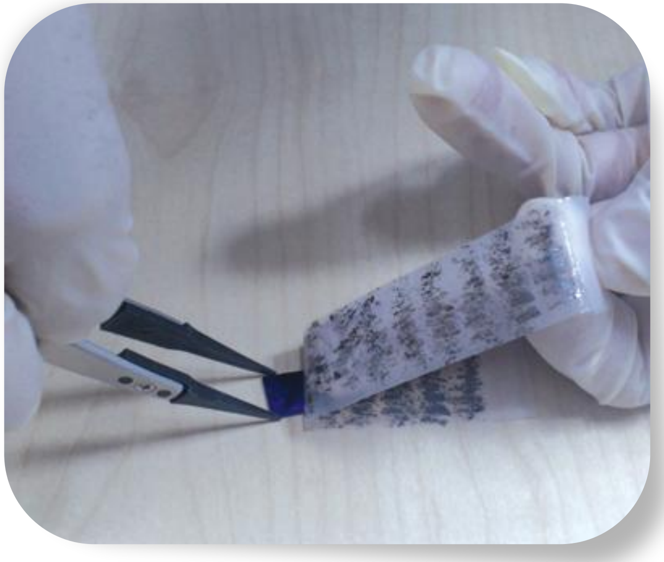
Figure 1 | Electrical resistivity of graphene as a function of temperature and doping (ρ, electrical resistivity; T, temperature; n, carrier density). Left panel: first-principles results obtained using a combination of density-functional perturbation theory, many-body perturbation theory and Wannier interpolations to solve the Boltzmann transport equation. Right panel: experimental data. Adapted from ref. 4, American Chemical Society.

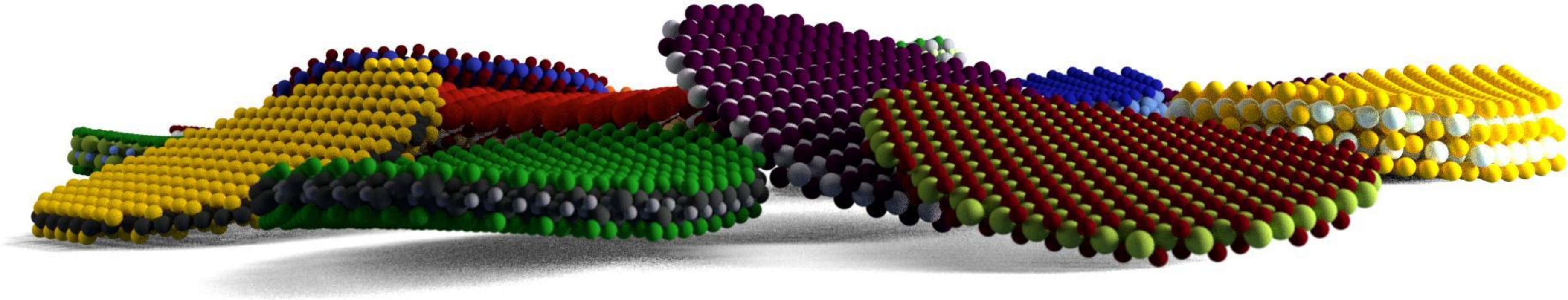
C.-H. Park *et al.,* Nano Letters (2014)
T. Y. Kim, C.-H. Park, and N. Marzari, Nano Letters (2016)

Technology stack for materials discovery

- **MaX quantum engines**
- An **operating system** for high-throughput computational science http://aiida.net
- A **dissemination platform** https://www.materialscloud.org/

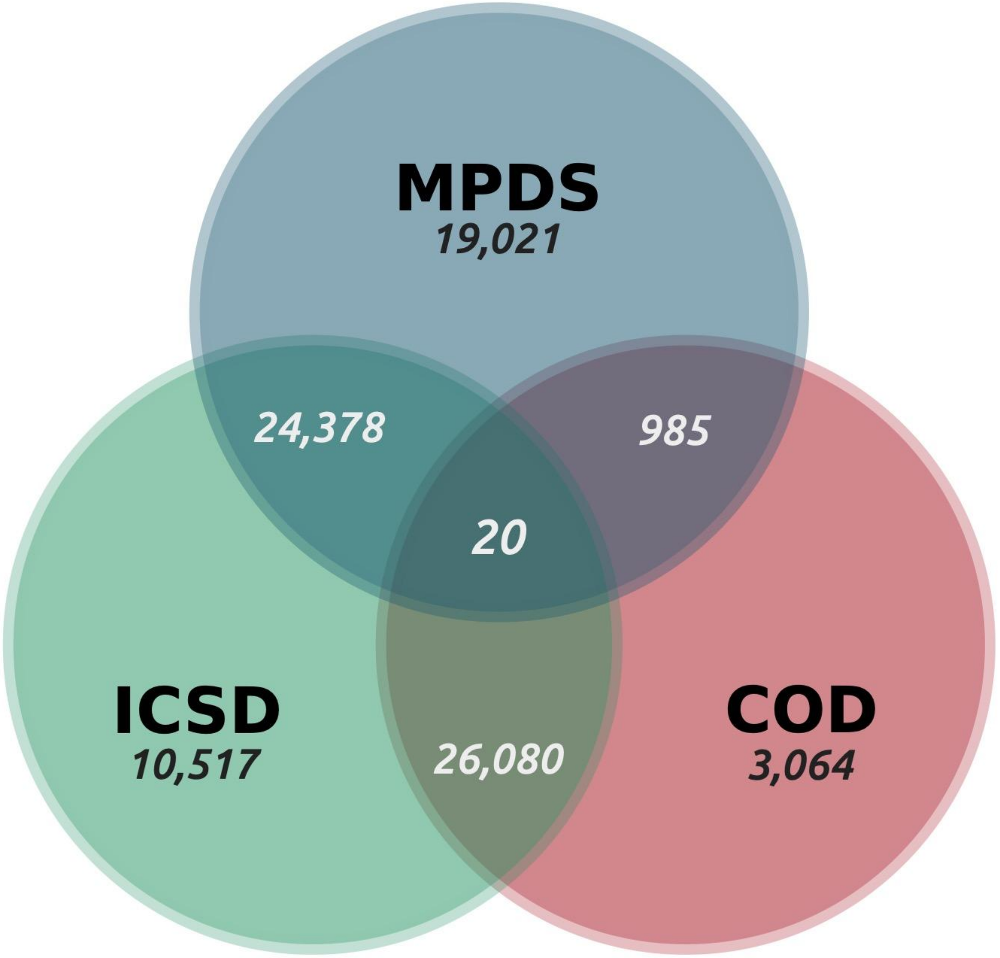
Computational exfoliation of all known inorganics





All known stoichiometric inorganics

TOTAL: ***84,065***

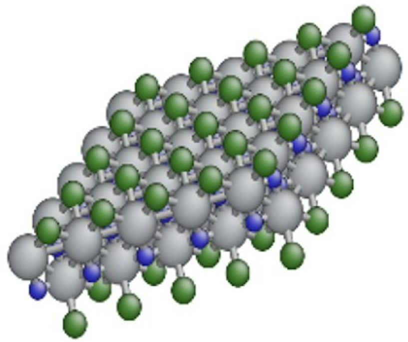


High-throughput funnel

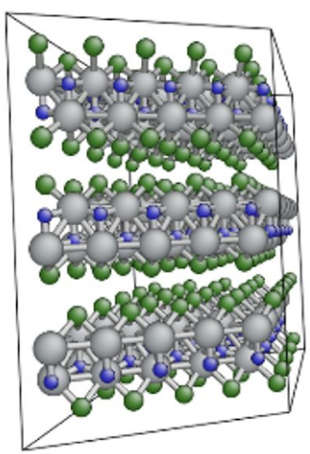
Exfoliation

External databases (ICSD, COD)

Geometrically layered



VdW-DFT electronic structure, binding energies



Characterization

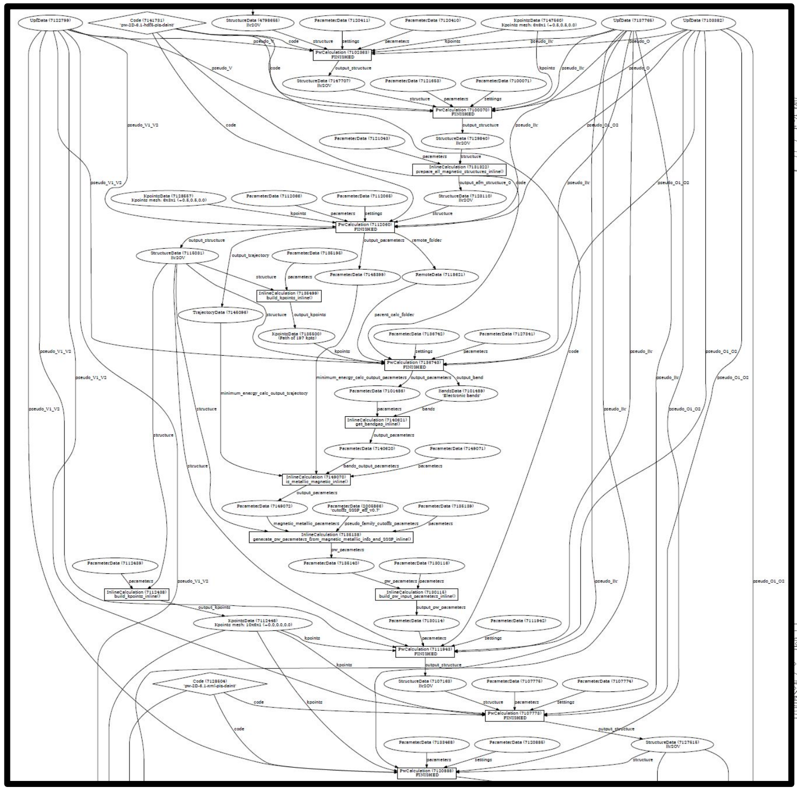
- Electronic
- Magnetic
- Mechanical

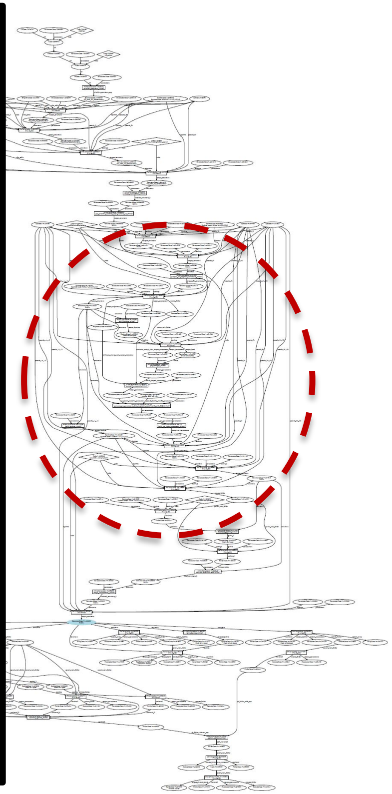
Applications

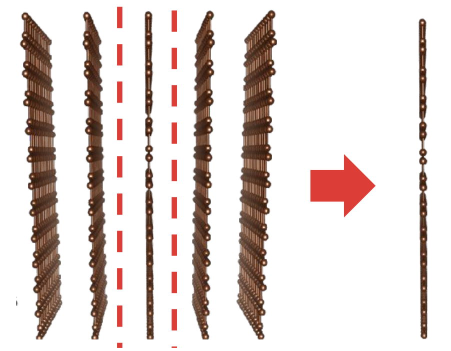
- High e/h mobility
- Topological
- CDW, spintronics
- Plasmonics
- Photocatalysis
- Membranes
- ....

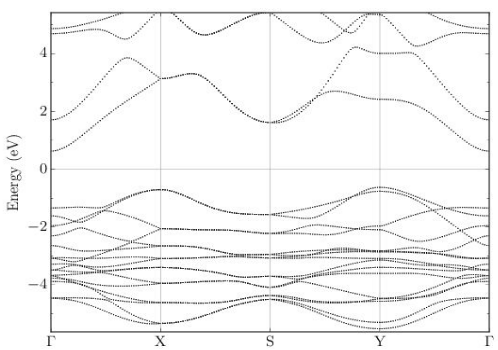
See also: S. Lebègue *et al.*, PRX (2013); R. Hennig *et al.*, PRL (2017) and E. Reed *et al.*, Nano Letters (2017), K. Choudhary, F. Tavazza, et al. Sci. Rep. (2017), and K. Thygesen, 2D Materials (2018)

Automated, reproducible workflows with full provenance

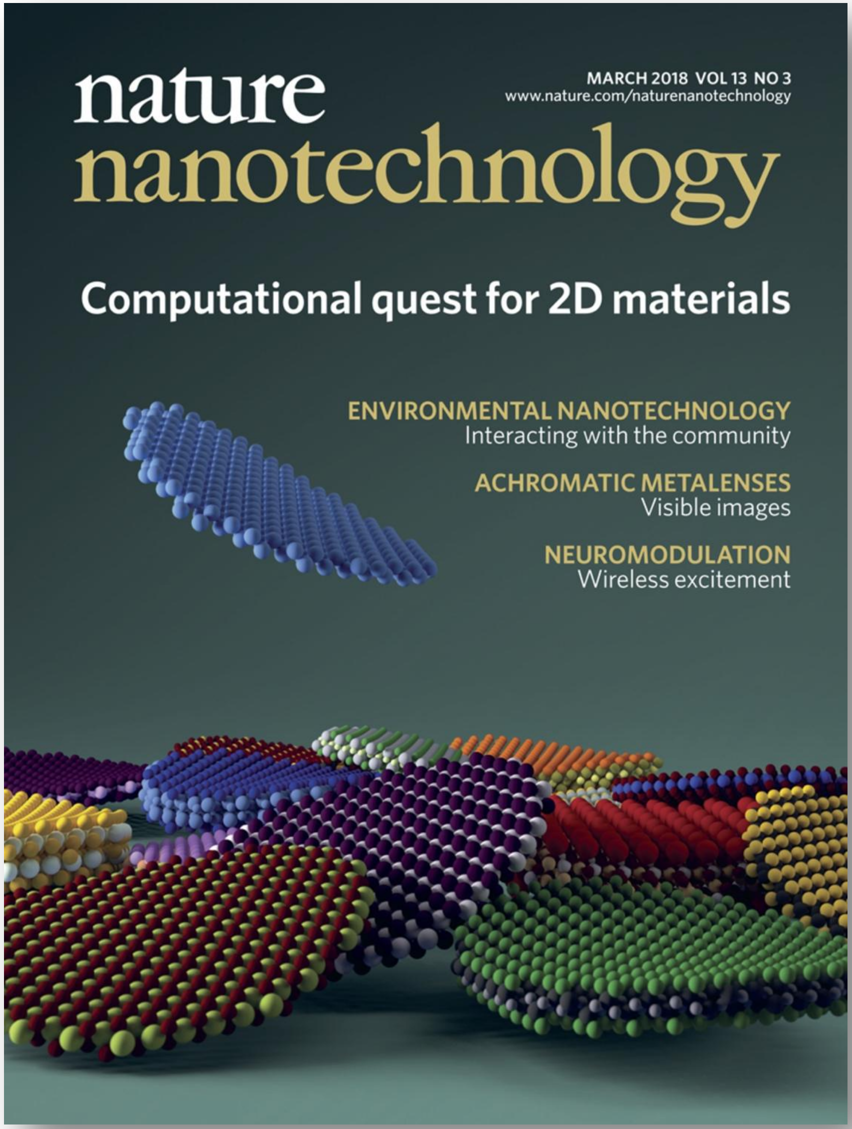








1800 novel two-dimensional materials



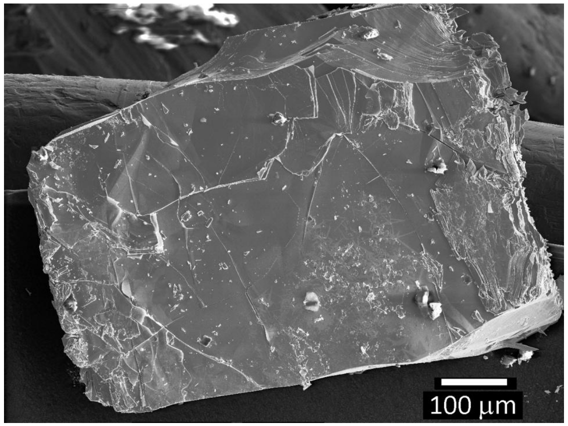
- High electron/hole mobility devices
- Topological insulators, quantum computing
- Ferromagnetic/spintronics in 2D
- Charge-density waves and superconductors
- Plasmonics, transparent conductors

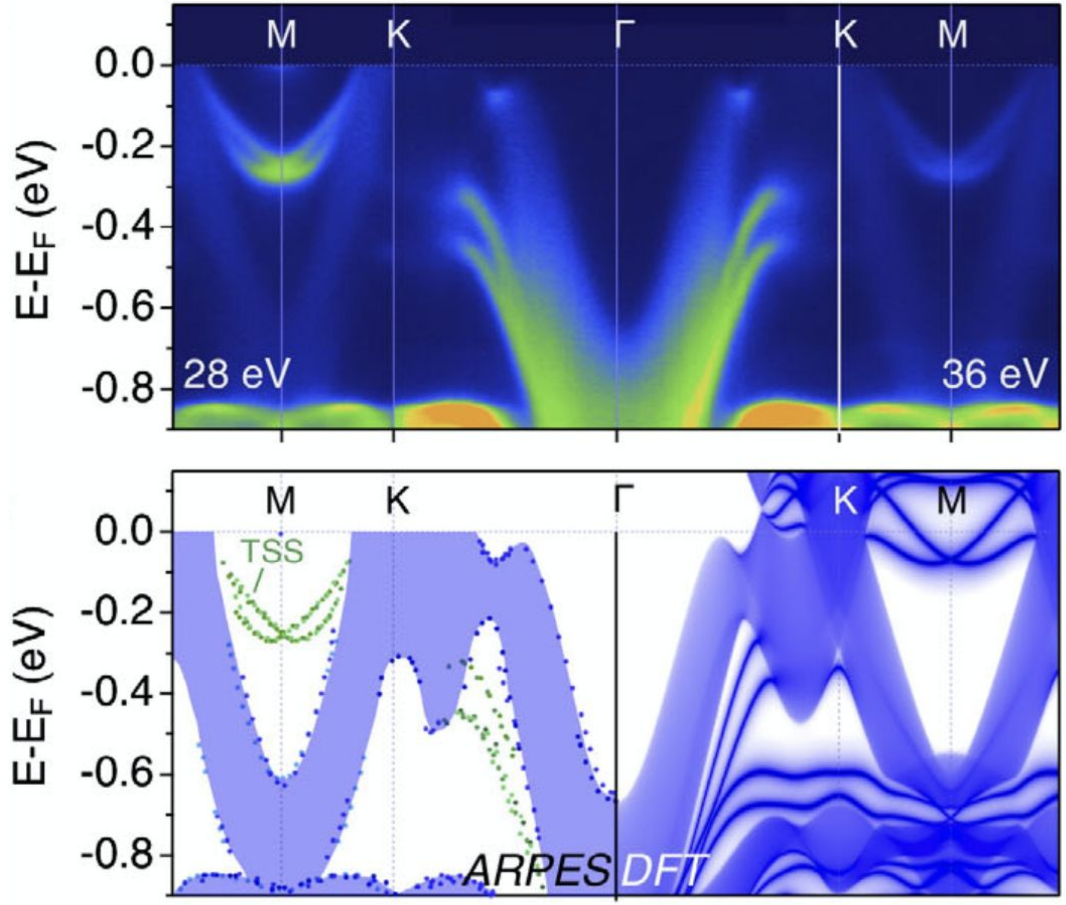
3D layered parents:

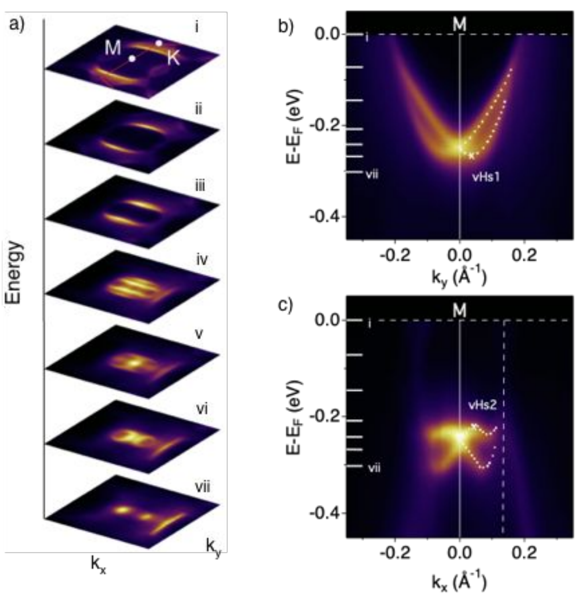
- Solid-state ionic conductors
- Hydrogen or oxygen evolution catalysts
- Membranes for filtration/separation
- Piezo, ferro, and thermoelectrics

N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, I. E. Castelli, A. Cepellotti, G. Pizzi and N. Marzari, Nature Nanotechnology 13, 246 (2018)

Jacutingaite: room-temperature Kane-Mele QSHI

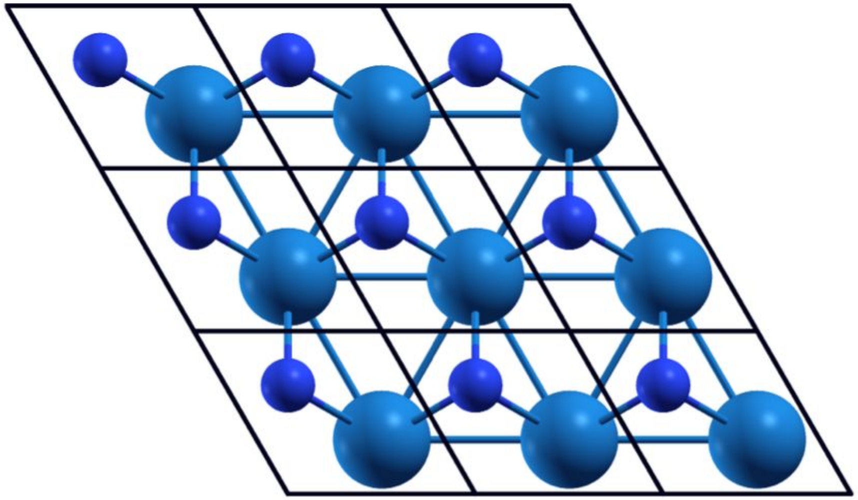


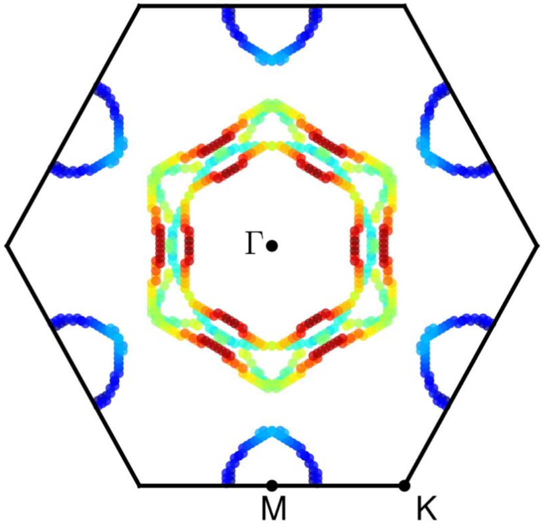


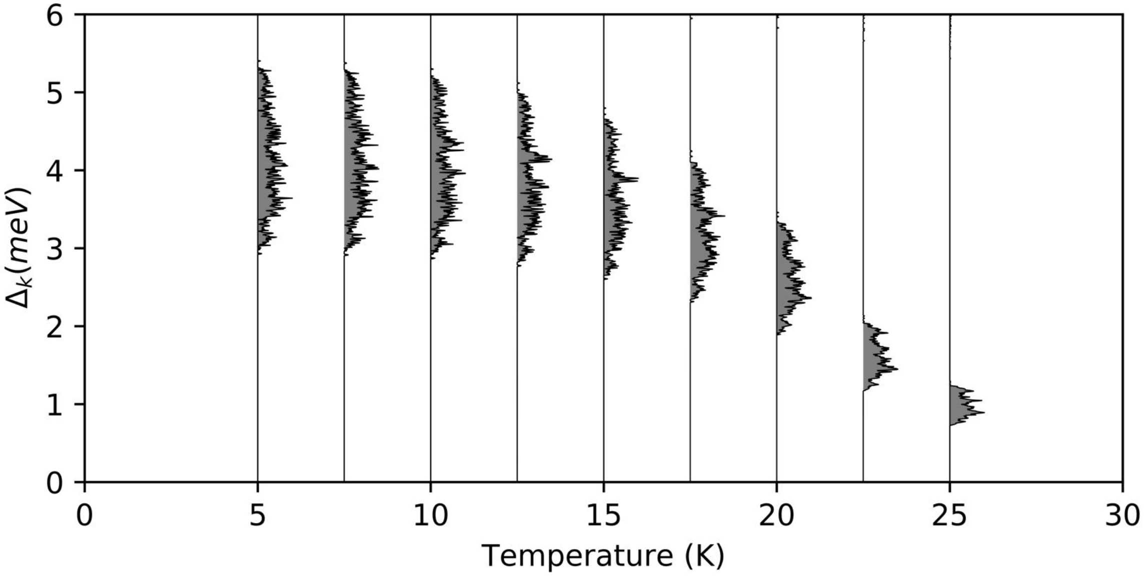


. Marrazzo *et al.,* Phys. Rev. Lett. 120, 117701 (2018)
I. Cucchi *et al.,* Phys. Rev. Lett. 124, 106402 (2020)
A. Marrazzo, N. Marzari, and M. Gibertini, Phys. Rev. Res. 2, 012063(R) (2020)

W_2N_3 : 27K superconductor in 2D





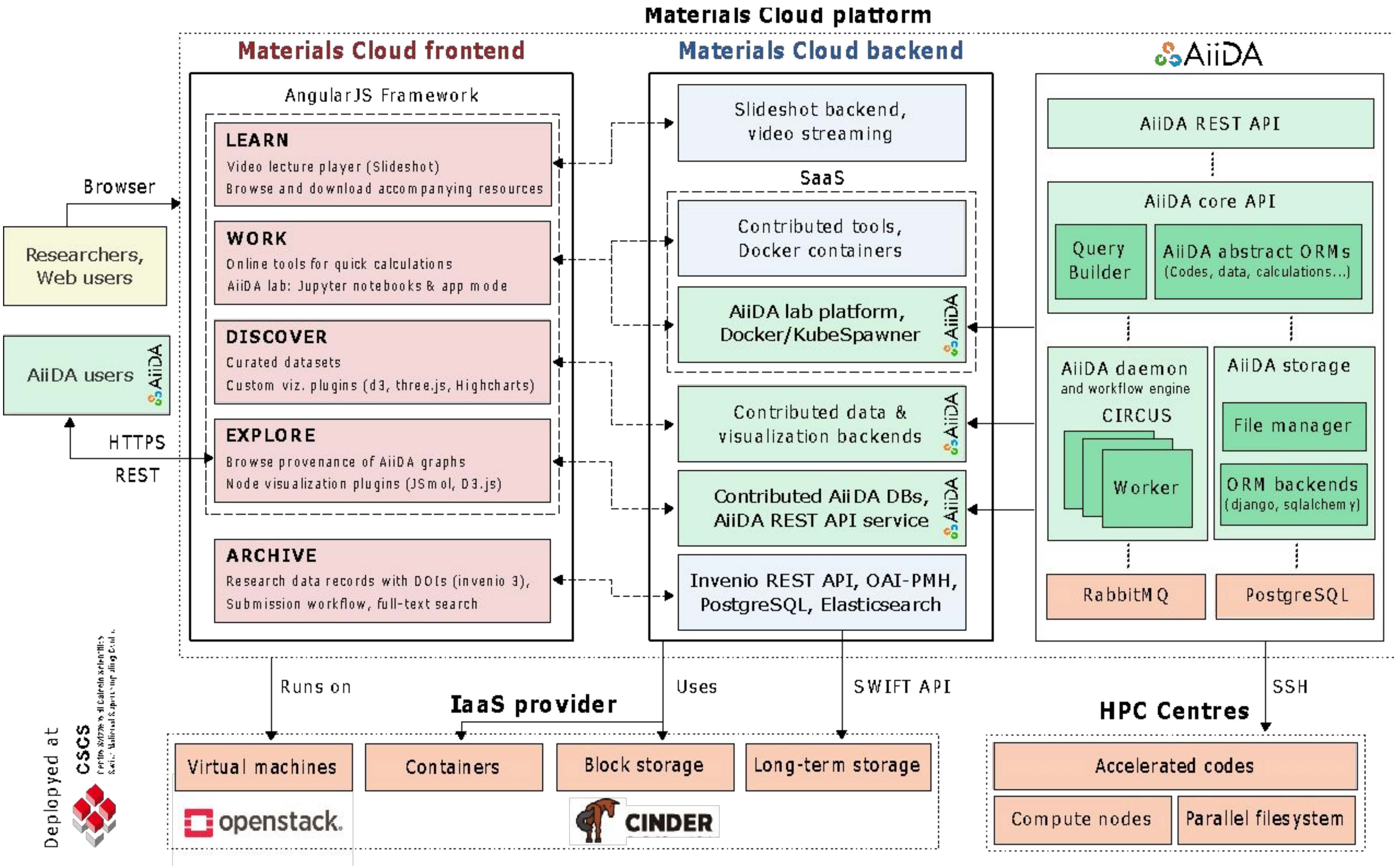


Automation Data Environment Sharing

http://www.aiida.net

S.P. Huber *et al.,* Nature Scientific Data (2020)
G. Pizzi *et al.,* Comp. Mat. Sci. (2016)

https://materialscloud.org



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Conclusions

- Materials enable the technologies that power our economy and sustain our society
- We can predict materials properties, and discover new materials, with first-principles simulations
- Ready for pre-exascale machines - 100,000 first-principles workflows/hour

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THANKS