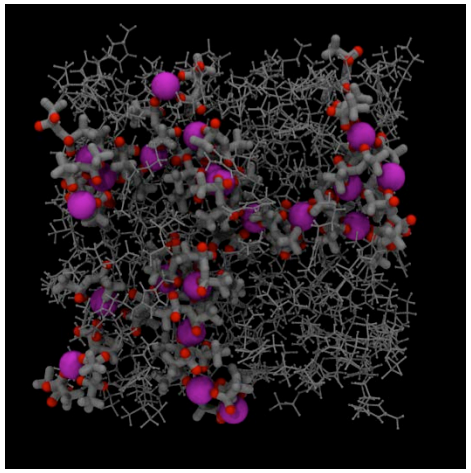
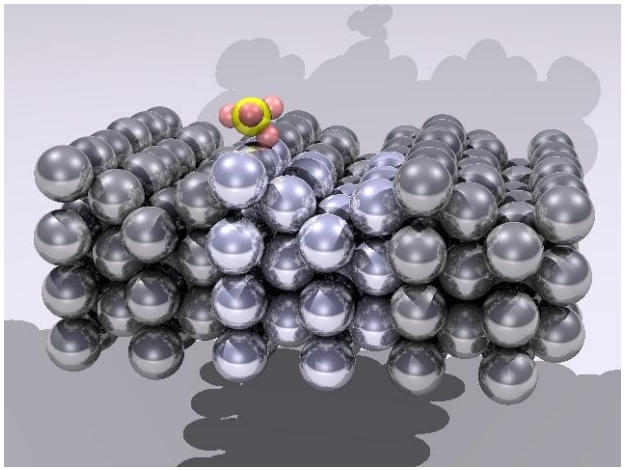
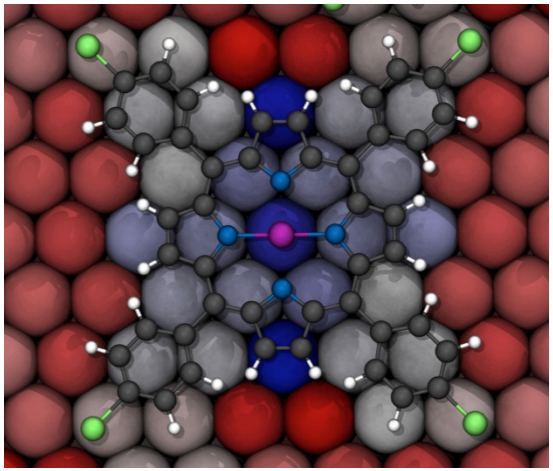
MATERIALS' REVOLUTION: COMPUTATIONAL DESIGN AND DISCOVERY OF NOVEL MATERIALS

EPFL-ETHZ-UNIBAS-UNIFR-UNIGE-USI-UZH-IBM-CSCS-EMPA-PSI

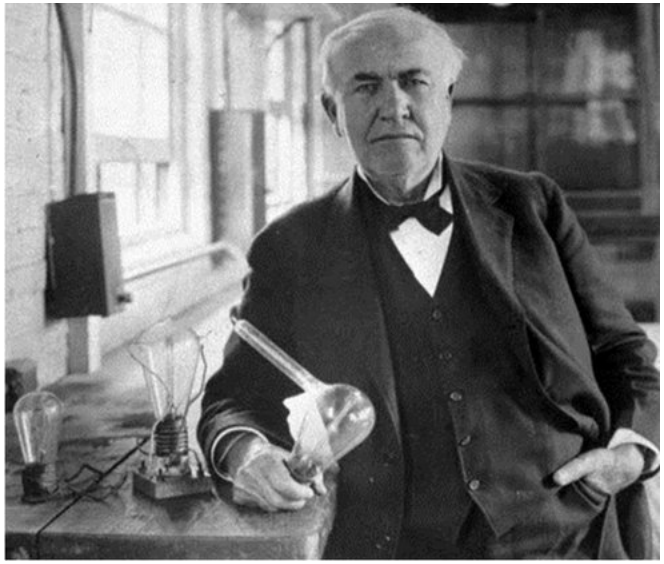






MATERIALS' DEVELOPMENT STILL EDISONIAN: INTUITION, SEARCHES, AND SERENDIPITY

- Edison tested 3000 materials for his filament – settling on burned sewing thread.



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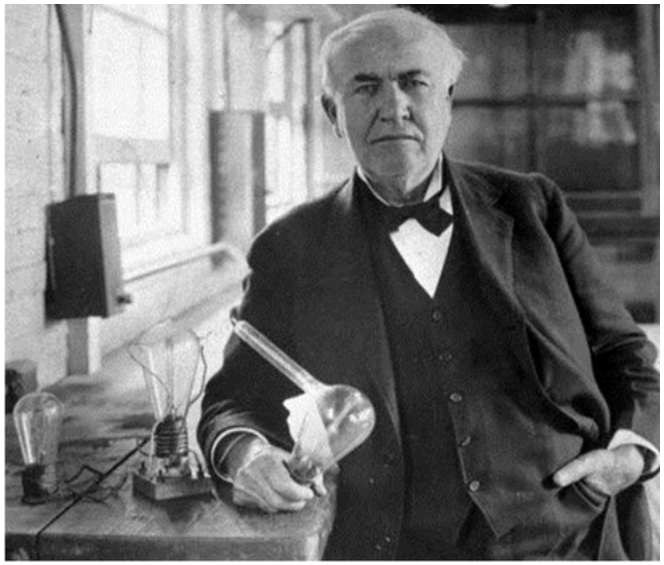

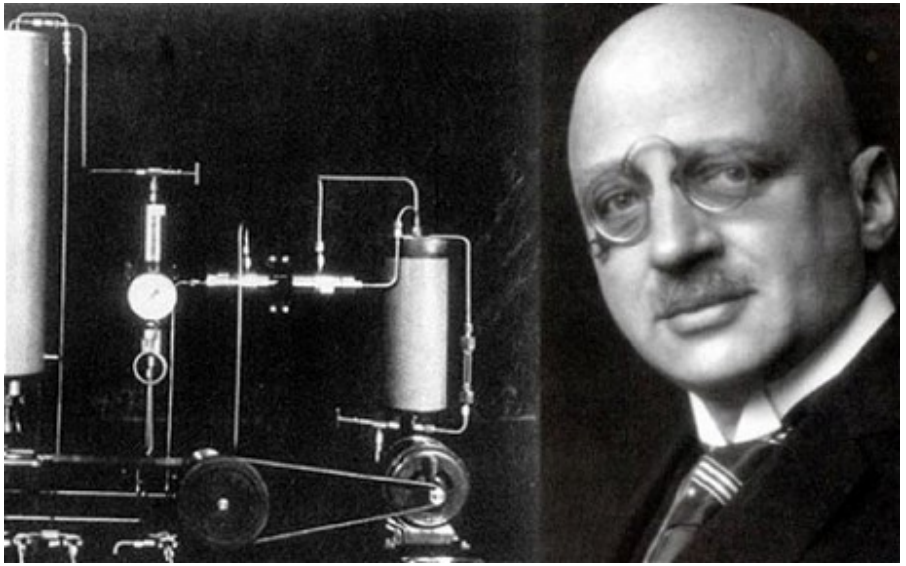

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- Norskov showed in 2009 that CoMo is a more efficient

nature chemistry
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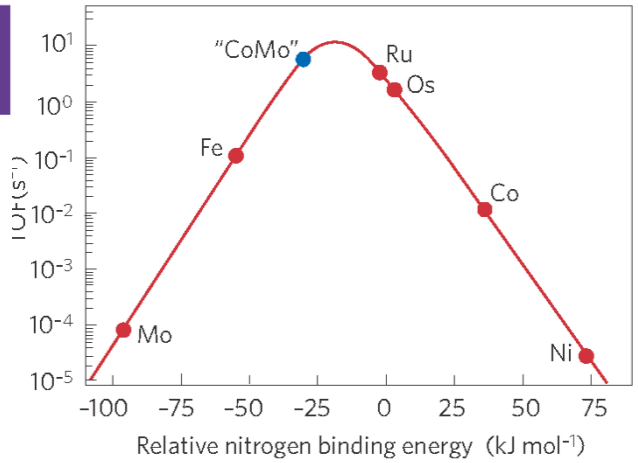
Towards the computational design of solid catalysts

J. K. Nørskov[1]*, T. Bligaard[1], J. Rossmeisl[1] and C. H. Christensen[2]



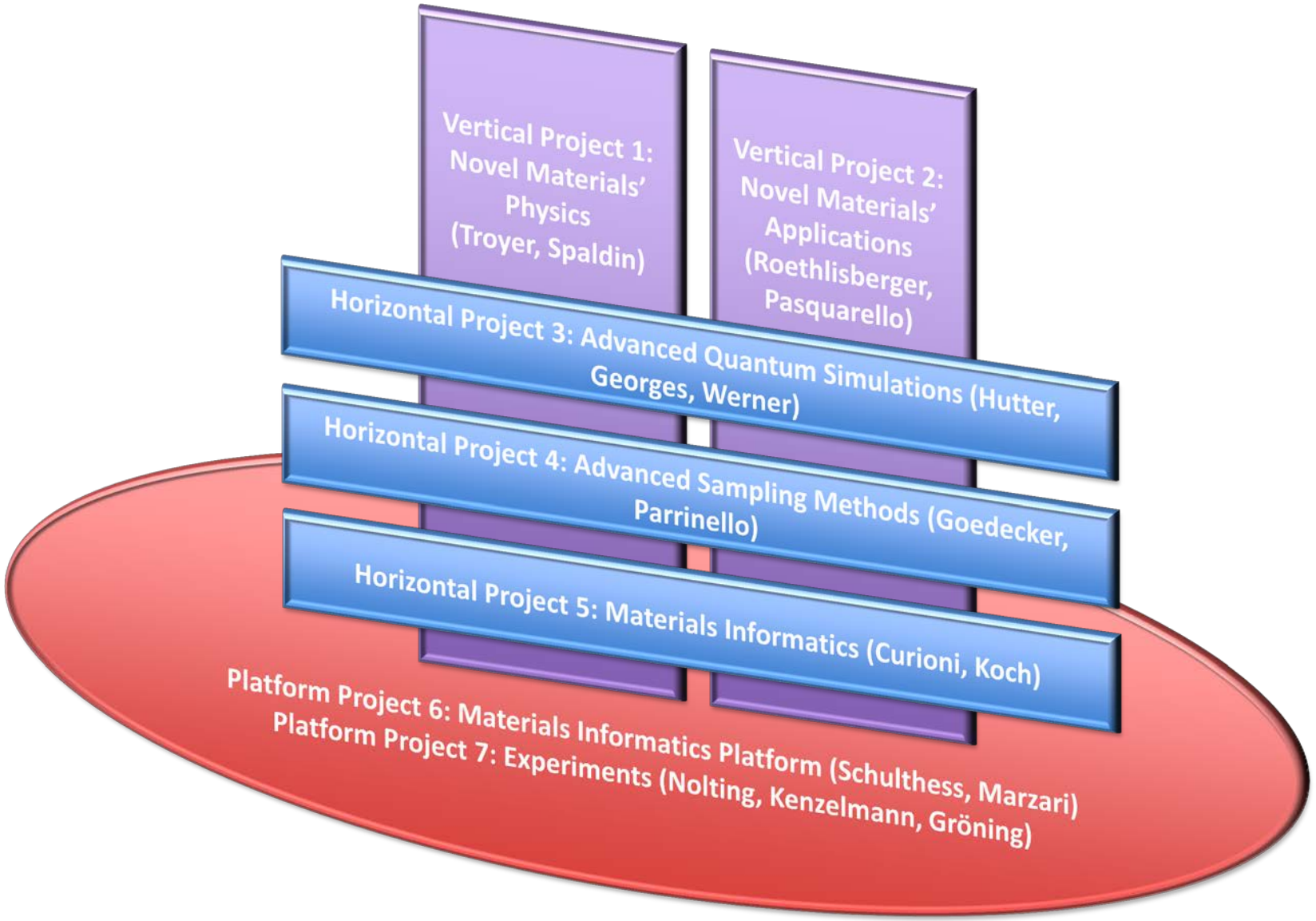
QUANTUM SIMULATIONS

- Accurate, hence predictive
- Can deal with the complexity of realistic systems
- Fast (total energies of all known inorganic materials: a couple of weeks)

MATERIALS DESIGN AND DISCOVERY

- Greatly accelerate the Edisonian approach…
- … and merge with the tools and concepts of computer science
- Push the state-of-the-art in quantum simulations
- Develop the methods/codes/systems for fast turnaround time on complex properties

NCCR SCIENTIFIC STRUCTURE



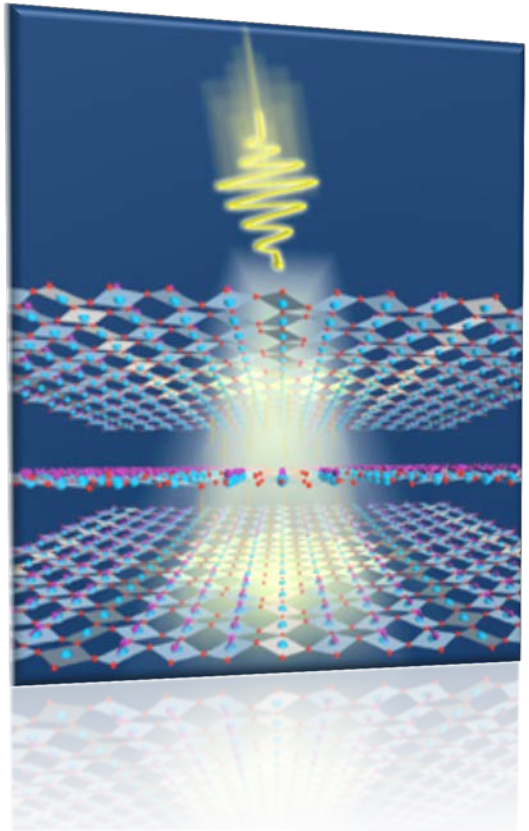
NCCR TEAM

EPFL (Marzari, Pasquarello, Roethlisberger, Koch, Corminboeuf, Yazyev), ETHZ (Spaldin, Troyer, VandeVondele), Basel (Goedecker, Von Lilienfeld), Fribourg (Werner), Geneva (Georges), Svizzera Italiana (Parrinello), Zurich (Hutter), IBM (Curioni), CSCS (Schulthess), EMPA (Groning, Passerone), PSI (Kenzelman, Nolting)

VP1: NOVEL MATERIALS PHYSICS (TROYER, SPALDIN)

Materials where the fundamental physics and resulting properties are driven by strong, correlated electronic interactions or complex electronic states.

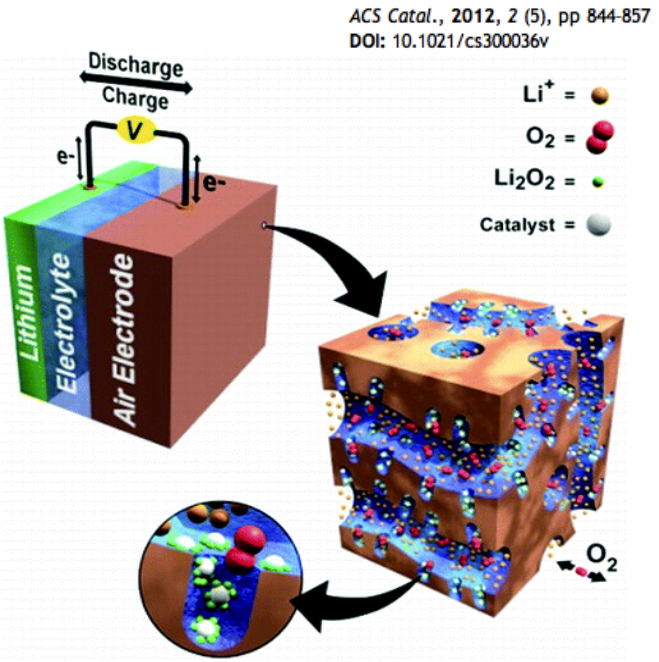
a) Multiferroics
b) Artificial heterostructures
c) Topological insulators
d) Model Hamiltonian materials
e) Dynamically excited materials



VP2: NOVEL MATERIALS APPLICATIONS (ROETHLISBERGER, PASQUARELLO)

Materials where quantum simulations are already accurate and predictive, and the search is over composition, structures, optimal performance.

a) Dye-sensitized solar cells
b) Photochemical water splitting
c) Metal-air electrochemical cells
d) Thermoelectrics



PP7: EXPERIMENTAL PLATFORM

- EMPA and PSI at the synthesis-and-characterization end of design pipeline
- Complemented by expt. University pole