us-eu bridging research efforts

Theory, Simulation and Modeling

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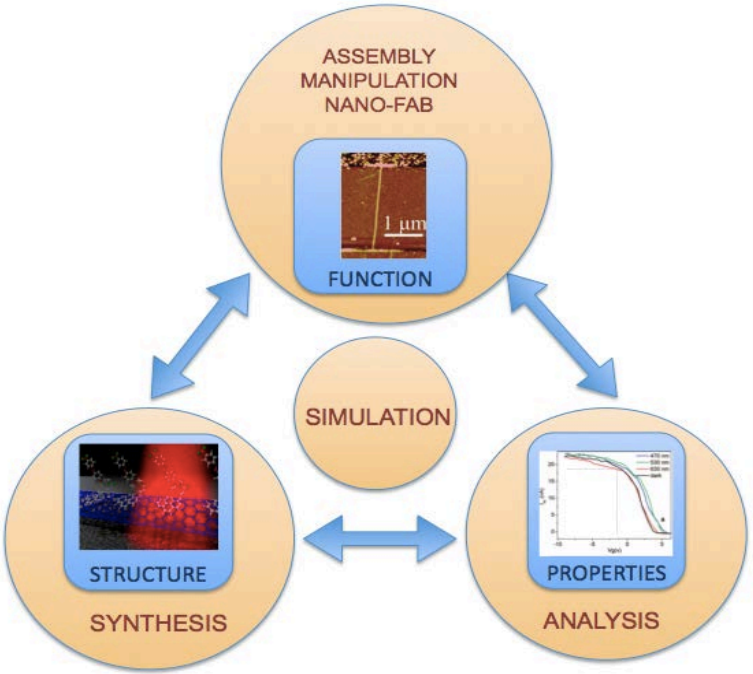
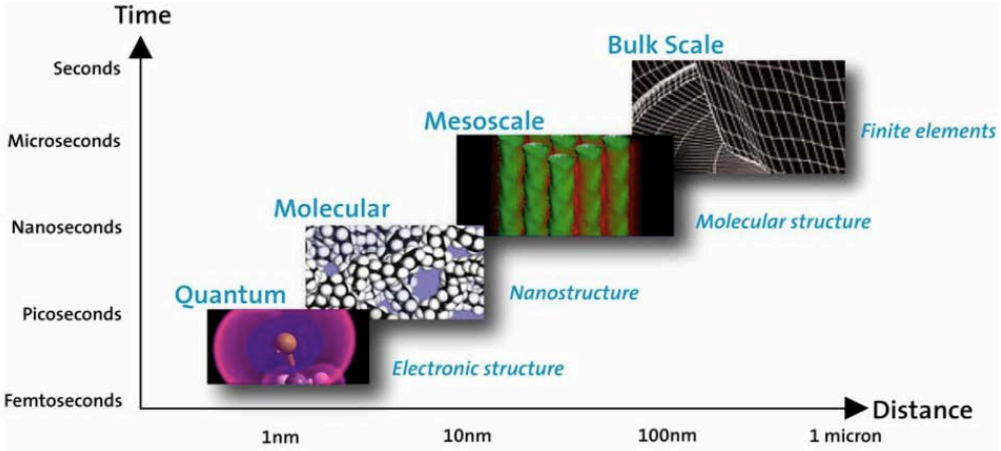
- **In which areas the multi-scale and multi-physics approach is the most advanced and could lead to a versatile multi-purpose modelling platform?**
  - Advanced (Nano) Materials - Devices
  - Bio - Nano interface
  - Interaction of nanostructures with light (and other excitations: photons, plasmons, phonons)
- **On which of the grand societal challenges would this modelling platform have the largest impact?**
  - Energy
  - ICT
  - Environment and Safety (Nanoparticles, chemicals)
  - Health
- **In which areas a EU-US collaboration is most likely to be successful in the short to mid-term?**
  - Code Standards - Interoperability - Libraries of tools - I/O standards - Passing info between scales
  - Defining protocols for databases, and sharing contents of computed materials properties
  - Exploiting Petascale and future (?) Exascale computers

Advanced Materials

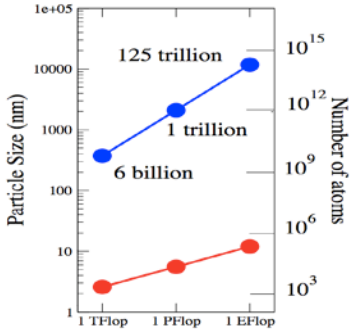
From atoms to devices





Force Fields
O(N)

Quantum
(Ab-initio)
$O(N^3)$



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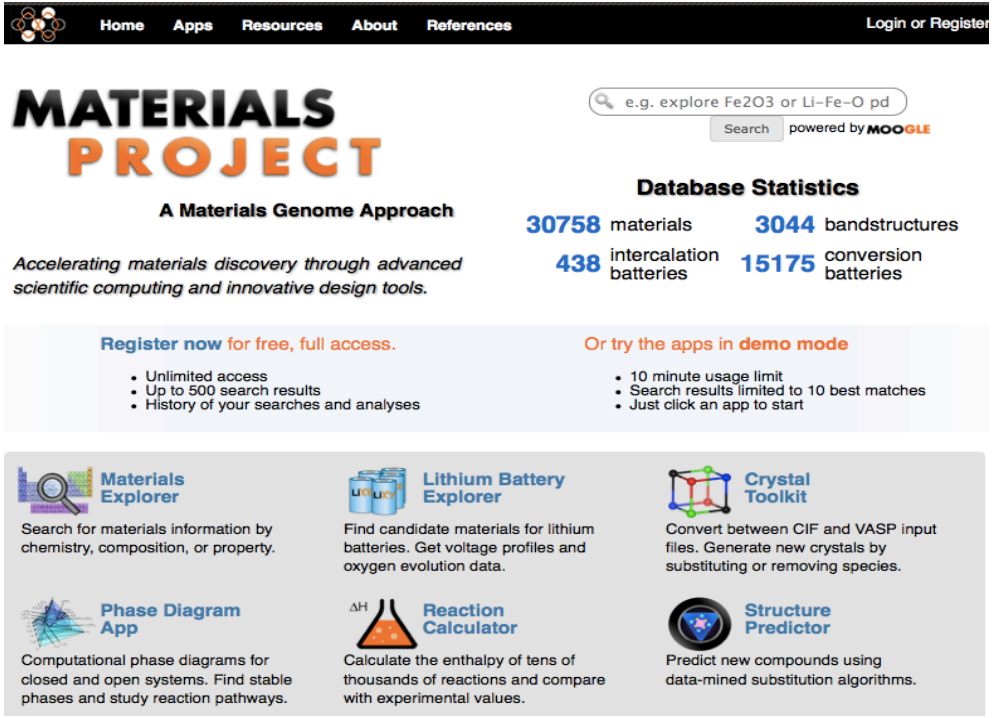
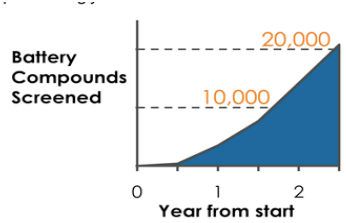
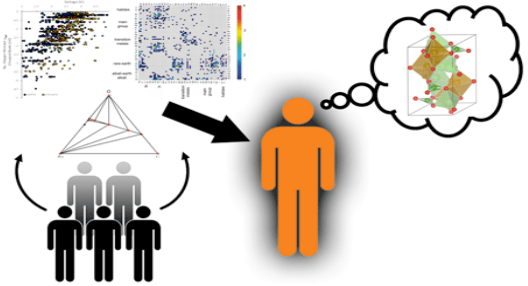
An example: The Materials Project

A Database of Materials Properties from a massive set of Ab-Initio calculations (MIT)







https://materialsproject.org/

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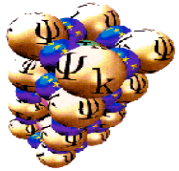
US - EU Collaboration

- Europe is very strong in Development of Materials Simulation Codes ("ab-initio": CP2K, VASP, SIESTA, WIEN2K...), with very successful Long-Term Collaborative Networks

EUROPEAN SCIENCE FOUNDATION
SETTING SCIENCE AGENDAS FOR EUROPE

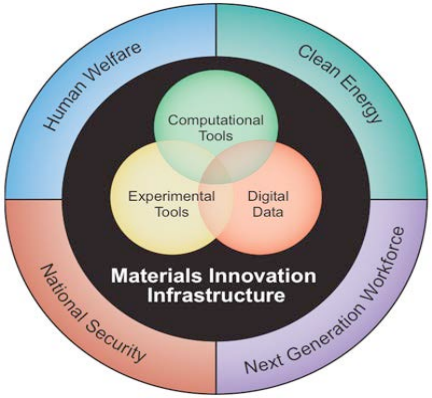


INTELBIOMAT

cecam
Centre Européen de Calcul Atomique et Moléculaire

- US is very strong in methodological development and final applications to grand societal challenges

Materials Genome Initiative



- Possibilities for collaboration:
  - Code Standards - Interoperability - Libraries of tools - I/O standards - Passing info between scales
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  - Exploiting Petascale and future (?) Exascale computers