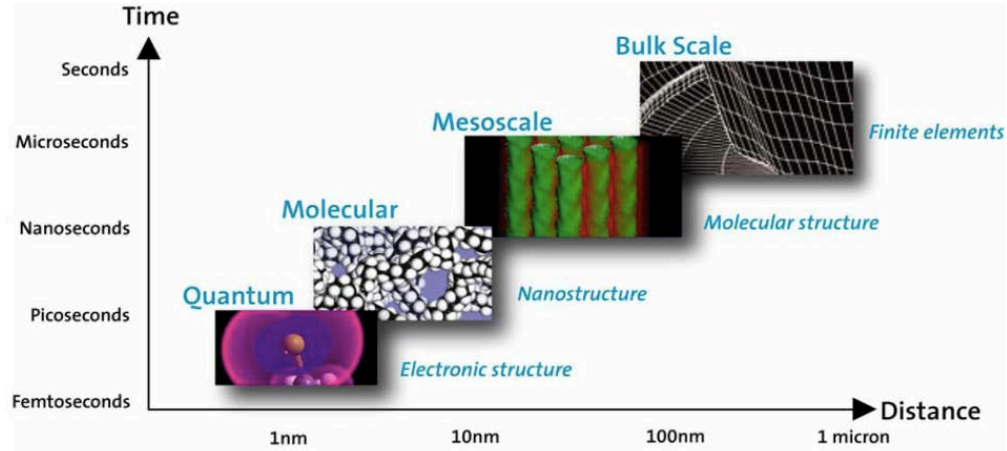
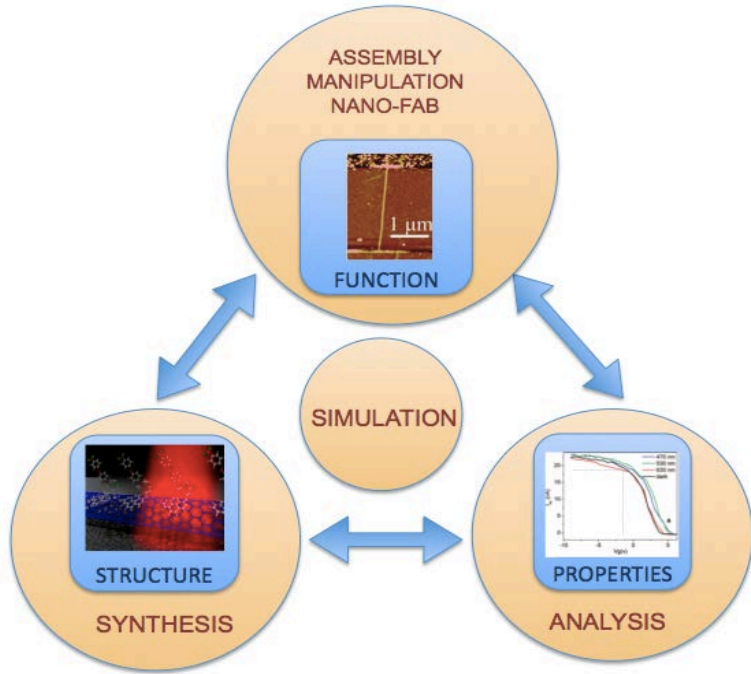


Pablo Ordejón, Director Institut Català de Nanociència i Nanotecnologia - ICN2

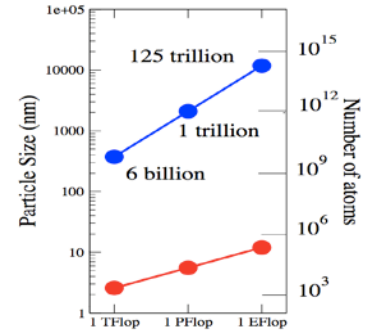
Barcelona, Spain - pablo.ordejon@icn.cat

- **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

From atoms to devices



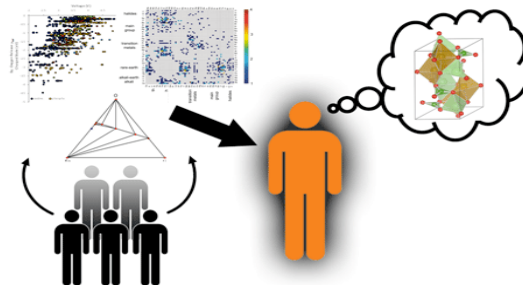
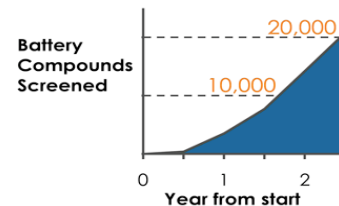
- Force Fields $O(N)$
- Quantum (Ab-initio) $O(N^3)$



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

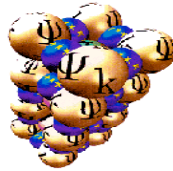
The screenshot shows the Materials Project website. At the top, there is a navigation bar with links for Home, Apps, Resources, About, and References, along with a Login or Register button. Below the navigation bar is the Materials Project logo and a search bar containing the text "e.g. explore Fe2O3 or Li-Fe-O pd". A search button and the text "powered by MOOGL" are also visible. The main content area features "Database Statistics" with the following data: 30758 materials, 3044 bandstructures, 438 intercalation batteries, and 15175 conversion batteries. Below the statistics, there are two options: "Register now for free, full access." and "Or try the apps in demo mode". The registration option lists benefits: unlimited access, up to 500 search results, and history of searches. The demo mode option lists limitations: 10 minute usage limit, search results limited to 10 best matches, and a simple click-to-start interface. At the bottom, there are six application tiles: Materials Explorer, Lithium Battery Explorer, Crystal Toolkit, Phase Diagram App, Reaction Calculator, and Structure Predictor, each with a brief description of its function.

 **18 years**
to move materials
from **lab** to **market**



US - EU Collaboration

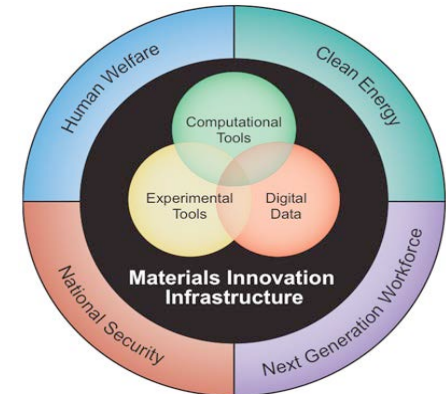
- Europe is very strong in Development of Materials Simulation Codes (“ab-initio”: CP2K, VASP, SIESTA, WIEN2K...), with very successful Long-Term Collaborative Networks



INTELBIOMAT



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



- Possibilities for collaboration:
 - 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