IPCMS

Institut de Physique et Chimie des Matériaux de Strasbourg

(presentation by Guido Ori)

- Strasbourg / Cronenbourg campus site
- 230 members
  - 80 Research & University staff
  - 60 Engineers & Technicians
  - 90 PhDs & Post-docs
- 5 departments (3 physics + 2 chemistry)
- Interest in the GDR by 3 members
- Area of expertise: Computational Materials Science
- CNRS section 15
- Activities in the 4th axe (Simulations/Théorie)

N A M E

GDR Nanomaterials for Energy Applications

ELABORATION
MEASUREMENTS & METROLOGY
SIMULATIONS & THEORY
APPLICATIONS

IPCMS

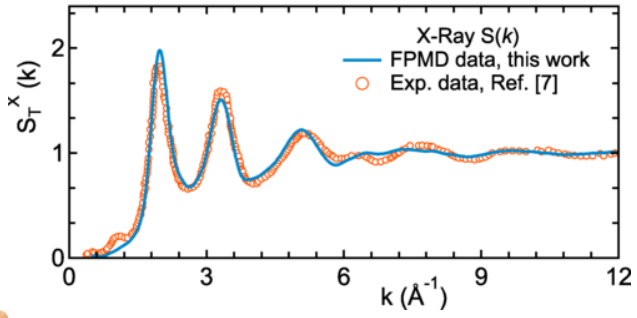
Institut de Physique et Chimie des Matériaux de Strasbourg

cnrs

Scientific expertise, overview, major themes in relation to the GDR

Scientific expertise in:

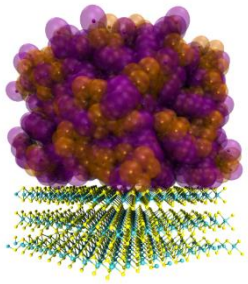
- Disordered (nano)materials:
  - Glasses: chalcogenides and oxides (PCMs & batteries)
  - Liquids: melts and ionic liquids (electr. devices, FETs)
- Hybrid (nano)systems:
  - Organic-inorganic interfaces: LSHs and IL@2Dmat
  - Glass-ceramics (cathode materials)

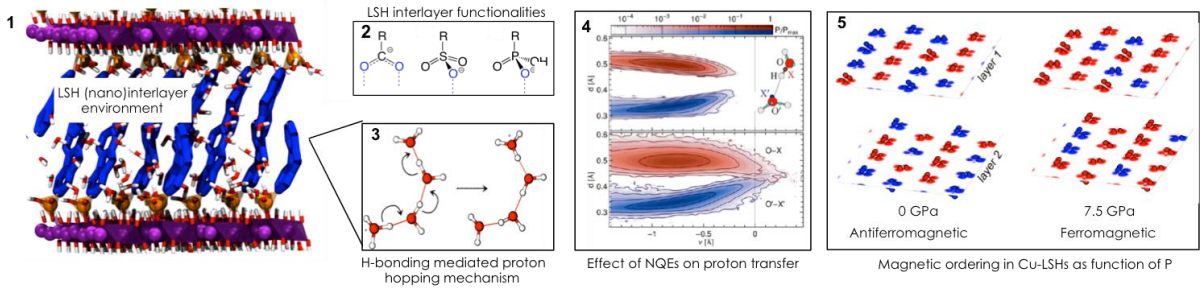


Phys. Rev. B 103, 094204 **2021**

Methodological expertise:

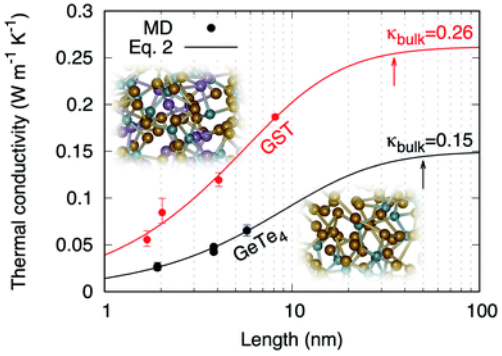
- First-Principles Molecular Dynamics (DFT-MD)
  - Code development (MB: CPMD, cp2k)
  - FES enhanced methods: metadyamics, BME
- Classical and Machine-Learned potentials MD
- Combined with AEMD (E. Martin team, iCUBE)





H-bonding mediated proton hopping mechanism — Effect of NQEs on proton transfer — Magnetic ordering in Cu-LSHs as function of P

Adv. Funct. Mater. 1703576, 1-13 **2017**



In collab. E. Martin team, iCUBE
RSC Advances 11, 10752 **2021**

Properties (qt.ve): Structure | Bonding / Electronic | Dynamics | Magnetic | Thermal