Service de Physique de l'Etat Condensé, SPEC/CEA-Saclay (Sawako NAKAMAE)

- ~60 researchers, +40 PhDs, ~15 PDs/alternance, 17 tech supp staff, 6 admin+IT staff.
  - ***Mesoscopic Physics and thermoelectricity***
  - ***Nanomagnetism and Oxides***
  - Quatronics
  - Nanoelectronics
  - Organics Electronics and Nanophotonics
  - Nanostructure and Surface Imaging
  - ***Out-of-equilibrium systems, hydrodynamics and Energy***
- 7 participants in GDR NAME
- Area of expertise of the labs
  - ***Thermoelectricity (mesoscopic & complex fluids)***
  - ***Solar-to-Hydrogen Conversion***
  - ***Ab initio simulations of electronic structure and quantum transport***
- CNRS and/or univ section: UMR 3680 and University Paris-Saclay
- Preferential axes: Elaboration, Property measurements, Simulation/Theory

N A M E

GDR Nanomaterials for Energy Applications

ELABORATION
MEASUREMENTS & METROLOGY
SIMULATIONS & THEORY
APPLICATIONS

spec

cnrs

Thermoelectricity: Mesoscopic systems & complex fluids

Mesoscopic thermoelectricity (theory/simulations)

- Phonon/Photon-assisted electronic quantum transport, 2D electron gas, graphene, nanostructures
- Heat carriers = Electrons, phonons
- Seebeck and Peltier thermoelectric effects
- Applications: Ultra-low Peltier cooling, quantum caloritronics, heat management in CPUs

μm, low T (1-100K), up to the GHz regime

Contact: genevieve.fleury@cea.fr

Complex fluids

- Thermoelectro-diffusion and electrochemical reactions
- Heat carriers = Ions and charged nanoparticles
- Energy conversion = Thermoelectric and thermogalvanic
- Application: Waste-heat recovery, storage and sensors

$1W/m^2$, $10mF/cm^2$

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Solar-to-Hydrogen Conversion

- Main research subject: Thin oxide films and oxide nanorods for solar water splitting
- Energy carriers: electrons
- Energy conversion type: photovoltaic, piezoelectric
- Applications: Solar energy storage in chemical bonds (e.g. H_2) using vastly abundant, inexpensive and environment friendly materials such as α-Fe_2O_3, $BaTiO_3$, etc.)

Objective: solar-to-hydrogen conversion efficiency > 10%

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DFT studies of quantum transport in nanostructures

- *Ab initio* (DFT, Density Functional Theory) based simulations for new materials and properties

- (Spin-polarized) electron transport, phonons:
  -- DFT + “tight-binding” (large scale) models

- Systems:
  -- Molecular junctions
  -- (Magnetic) molecules/substrate
  -- 2D materials and heterostructures

- Type of energy conversion: heat/charge, spin/charge

- Applications: low energy devices, sensors, etc.

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Technical or technological expertise in relation to the GDR issues

- What kind of materials/dimensions
  - Molecular junctions, molecules/substrate, 2D materials, semiconductor nanowires, etc
  - Nanofluids, ionic liquids (1-10mL)
  - Thin films (10 nm-100 nm), “Carpet-like” nanorod layers (ϕ ~ 50 nm, lengths ~100 – 400 nm)
- Bottom-up
- Elaboration techniques
  - Molecular beam epitaxy, aqueous chemical growth, lithography
- Characterization techniques
  - Thermoelectrochemical cells & generators
  - Photo-electrochemical cell, Synchrotron Radiation (Diffraction, absorption, microscopy)
  - Numerical methods: DFT, plane waves, localized orbitals; Green functions, scattering matrices, or real-time dynamics for quantum transport
- Special instruments or methods
  - Potentiostat, high-temperature liquid characterization station (200°C), …
  - Molecular beam epitaxy assisted by oxygen plasma, impedance spectroscopy modelization, AFM, ferroelectric test system
- Codes/numerical tools/modelling :
  - KWANT, t-KWANT
  - Quantum-ESPRESSO, Fireball.

Looking for collaborations? Visit us https://iramis.cea.fr/spec/

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