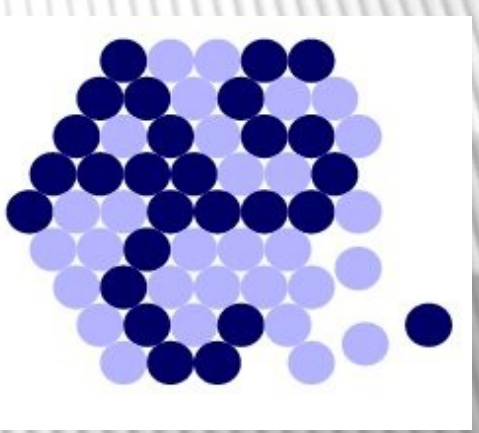
Queen's University Belfast



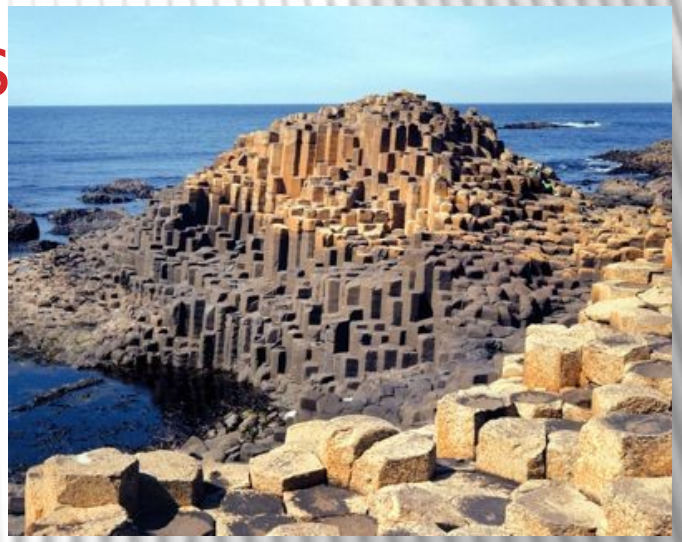
The Atomistic Simulation Centre

At Queen's University Belfast

Northern Ireland

Click to edit Master text styles

- Second level
  - Third level
    - Fourth level
      - Fifth level



What do we do?

- **We develop and use computational and theoretical methods to study structural, dynamical and electronic properties of molecules and nanostructures, solids, liquids, plasmas at the atomic scale.**

- **We study inter-disciplinary problems at the interfaces between Chemistry, Condensed Matter, Nanotechnology, Materials Science, Biology and Engineering.**

- **We push the frontiers in:**
  - **electron transport in nanostructures;**
  - **irradiation of materials and biological matter;**
  - **laser-matter interactions with ultra-fast pulses**

Members

- Daniel Dundas (MP)
- Myrta Grüning (MP)
- Meilan Huang (CCE)
- Jorge Kohanoff (MP)
- Ian Lane (CCE)
- Jim McCann (MP)
- Lorenzo Stella (MP+CCE)
- Tchavdar Todorov (MP)
- Gareth Tribello (MP)

MP= Maths and Physics

CCE= Chemistry and Chemical Engineering

Associated Members

- Peijun Hu (CCE)
- Irina Tikhonova (Pharmacy)
- Saurav Goel (Mech. Eng.)

Related Groups

- CTAMOP (Atomic, Molecular and Optical Physics)
- QTEQ (Quantum

expertise

- Density functional theory and quantum chemistry (JK, IL, MG)
- Ab initio Molecular Dynamics (JK)
- Many-body theory: GW and Bethe-Salpeter equation (MG)
- Semi-empirical (tight-binding), QM/MM (JK, MH)
- Real-time electron dynamics: TDDFT (DD, MG, LS, JK, TT)
- Non-adiabatic dynamics: Ehrenfest and beyond (TT, DD, LS)
- Enhanced sampling and automated analysis of trajectories in Molecular Dynamics (GT)
- Vibrations, phonons, quantum nuclei (TT, DD, LS, JK)
- Non-equilibrium MD: Generalized Langevin Equation (LS)

interests

CHEMISTRY: Ionic liquids, Crystallization, Mechanochemistry, Superhydrophobicity, Heat storage, Catalysis and Photocatalysis, Astrochemistry

BIOLOGY: Biomolecular dynamics, Pharmaceutical drugs, Radiation damage and radiotherapies.

NANOSCIENCE: Nanoelectronic/photonic/plasmonic devices

PHYSICS: Nuclear materials, Photovoltaics, Ferroelectrics.

ENGINEERING: Building materials, Stability of structures, Wearing of tools, Bubble technologies.

Codes maintained

EDAMAME: TDDFT on adaptive grids for laser-molecule systems.

THeREMIN: TDSE for laser interactions with H2+: electron-phonon correlation

H2MOL: TDSE for laser interactions with H2

YAMBO: Many-body electronic structure based on time-dependent non-equilibrium Green functions. Theoretical spectroscopy.

Poly-CEID: Non-adiabatic molecular dynamics on tight-binding electronic structure.

PLUMED: plugin for free energy calculations to use in conjunction with MD codes.

TBE: Self-consistent tight-binding molecular dynamics.

p-DINAMO: Correlated electron-nuclear dynamics.

Collaborations in Argentina

Existing and active:

Mario Del Popolo (Mendoza)

Sergio Koval, Jorge Lasave and Ricardo Migoni (IFIR)

Existing but inactive:

Dario Estrin (UBA)

In conversations:

Eduardo Bringa (Mendoza)

Valeria Ferrari (Tandar)

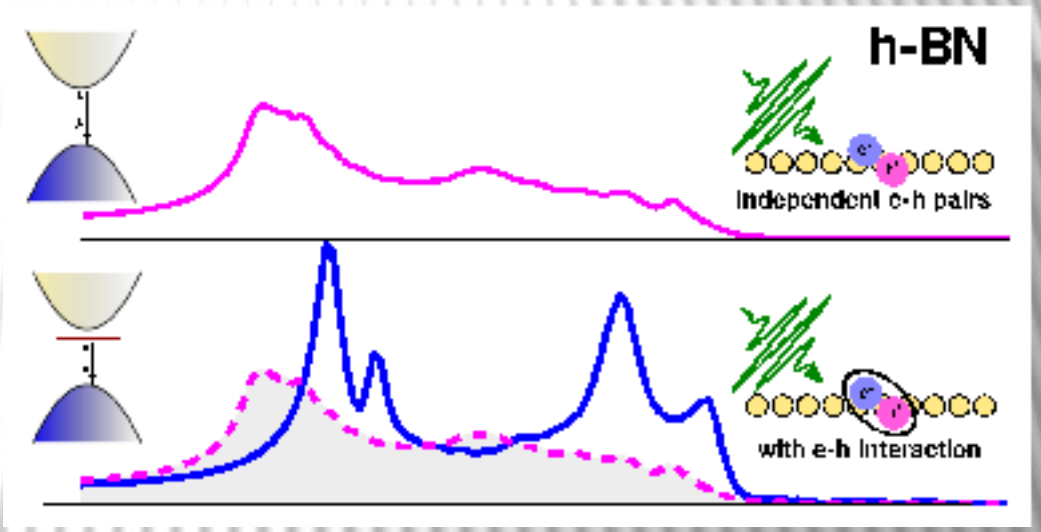
Paola Quaino (Santa Fe)

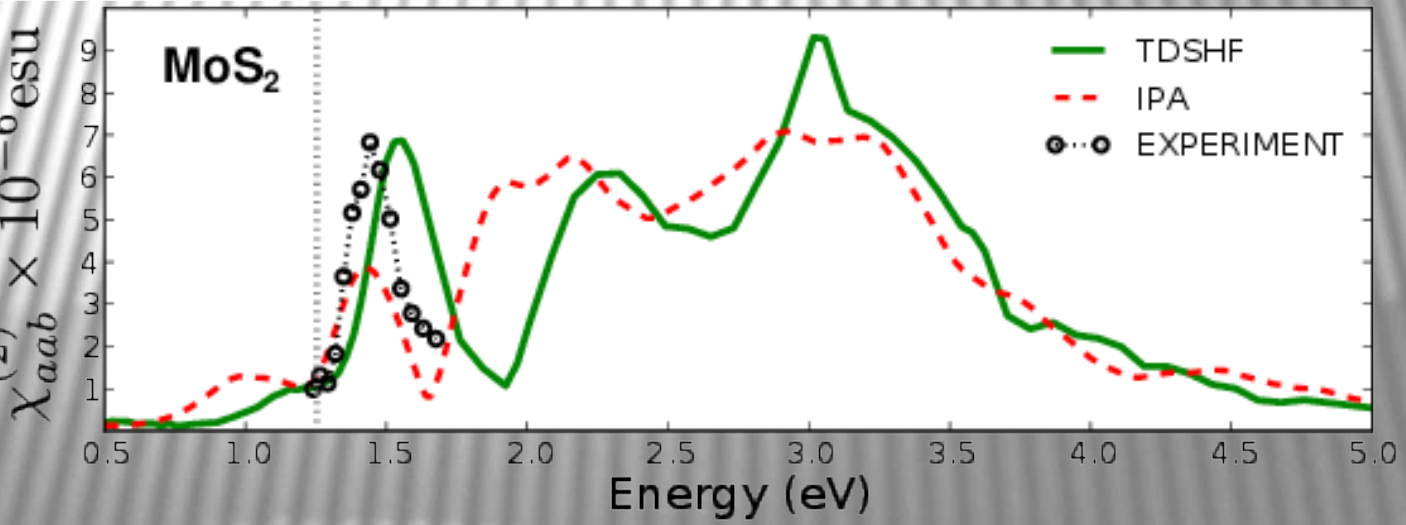
- **The whole group is open to consider other collaborations,**
- **also to receive people from RA with CONICET external fellowships,**
- **and to apply for funding, e.g. Royal Society, EU, RAICES-Siembra**

Photoinduced electron dynamics

Myrta Grüning

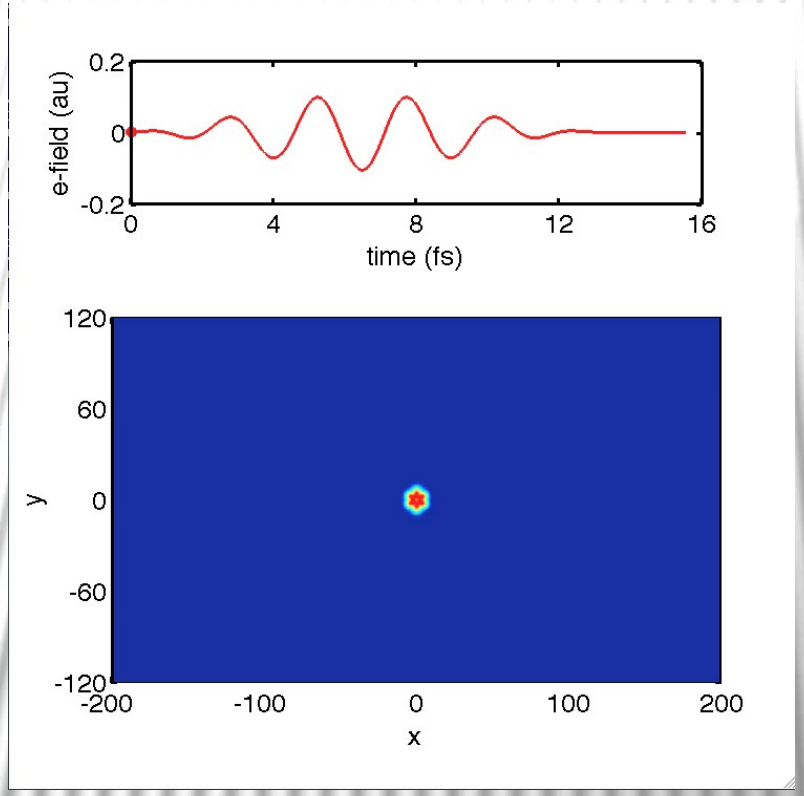
- **Ab initio real-time approach based on Green's function theory and DFT**
- **Nonlinear properties (e.g. SHG) including key many-body effects such as e-h interaction**
- **Focus on 2D graphene-like materials**





TDDFT: High harmonic generation

Daniel Dundas

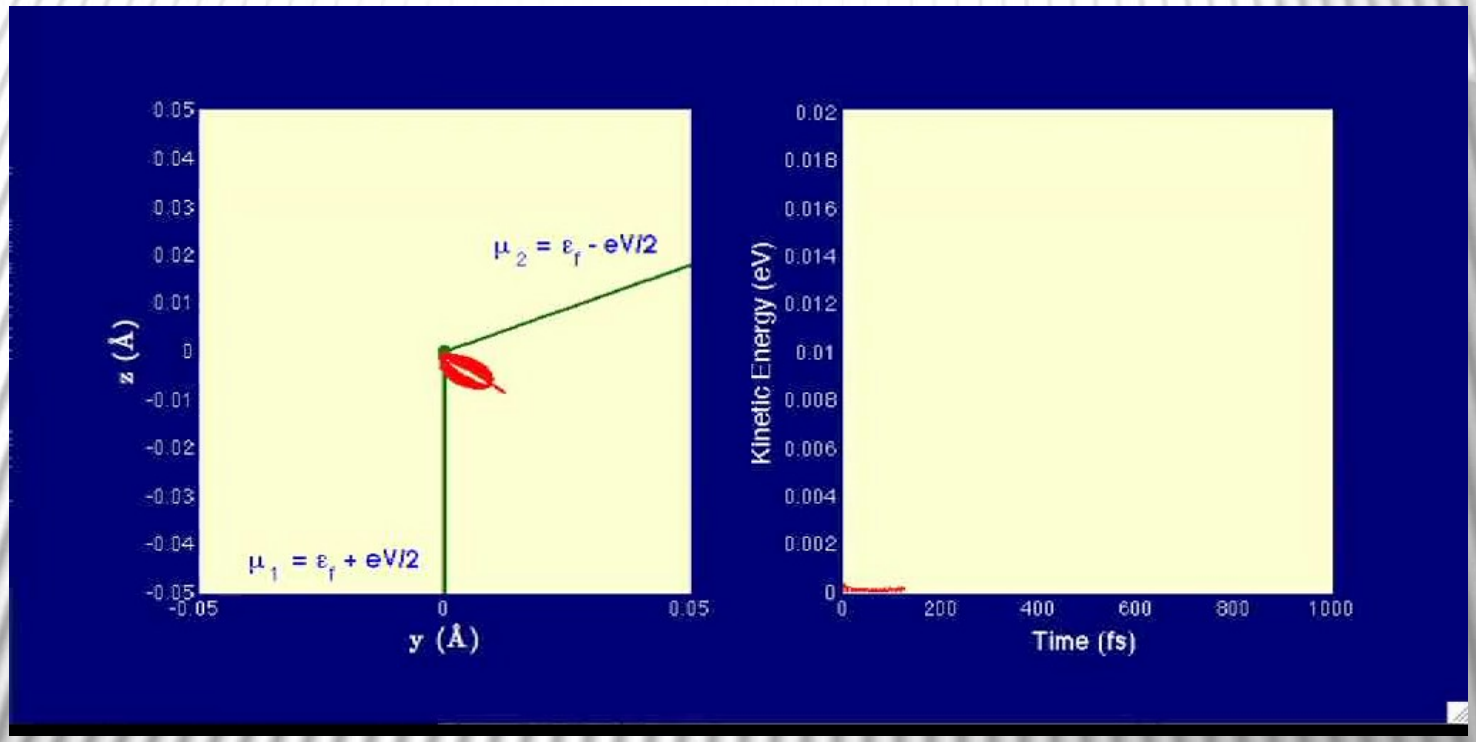


Ionization of Benzene by an intense, ultrashort laser pulse

The benzene molecule lies in the plane and the laser pulse is linearly-polarised with the polarization direction horizontal in the plane. Ionizing electron wavepacket is emitted each half-cycle, in anti-phase to the field.

Conduction in nanowires

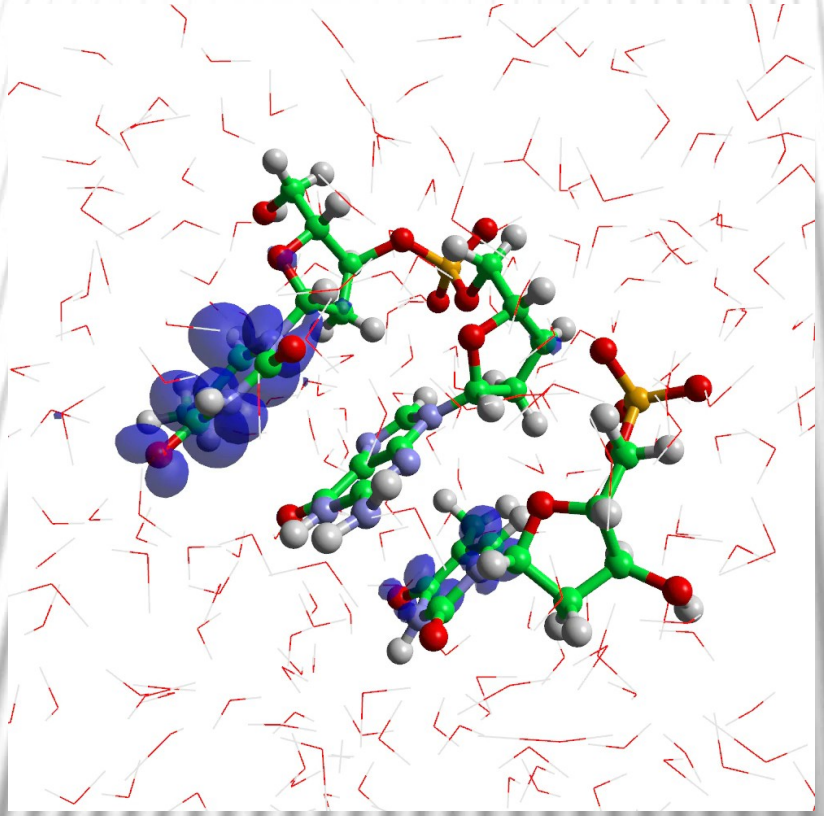
Tchavdar Todorov, Daniel dundas



Open-boundary non-adiabatic molecular dynamics simulation of the corner atom in a bent atomic wire. The atom is driven in an expanding orbit by the non-conservative current-induced force on it. This has been called the **atomic waterwheel effect**.

Dynamics of irradiation:
DNA damage by low energy electrons

Jorge Kohanoff



An initio molecular dynamics simulation of an **excess electron in a tri-nucleotide**. This is a metadynamics simulation where **a strand break is forced** but the program finds automatically where is more likely to happen, depending on the **base sequencing**.

Non-adiabatic dynamics

Lorenzo Stella

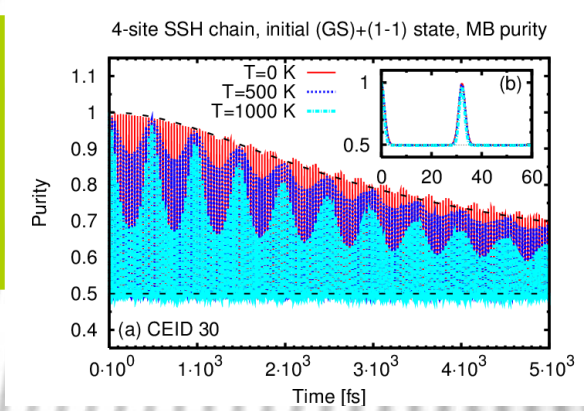
Correlated electron-ion dynamics (CEID)

Atomic motion + electronic transitions, Quantum electrons and ions

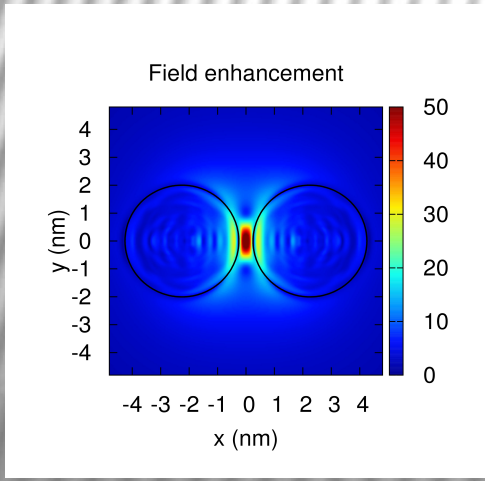
Deterministic (no "hops"), scalable (extending Eherenfest dynamics)

Competition between quantum coherence and dissipation

Model revivals in the electron purity decay (entanglement)

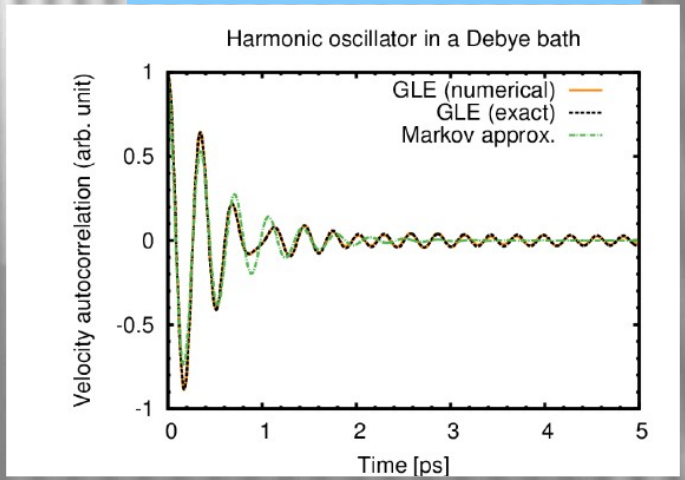


Generalized Langevin Equation. Improving the embedding of atomistic systems in structured environments



Quantum plasmonics

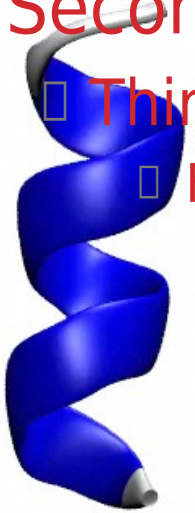
Exploring quantum non-locality in metallic nanostructures by TDDFT

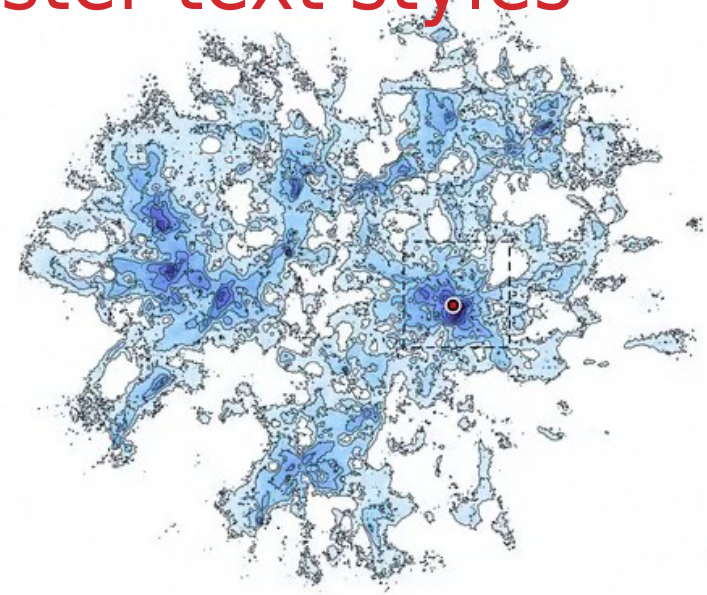


Analysis of MD trajectories

Gareth Tribello

- Click to edit Master text styles
  - Second level
    - Third level
      - Fourth level
        - Fifth level





Left: trajectory generated by a molecular dynamics of a short peptide (132 atoms). This data has an enormous dimensionality.

Right : using techniques we have developed we map each high-dimensional frame in the movie on the left to a 2-D vector. The red dot shows the location of the frames on the left in this map. This makes visualization and analysis much easier.

Chemical physics

Gareth Tribello, Jorge Kohanoff, Mario del popolo (Mza)

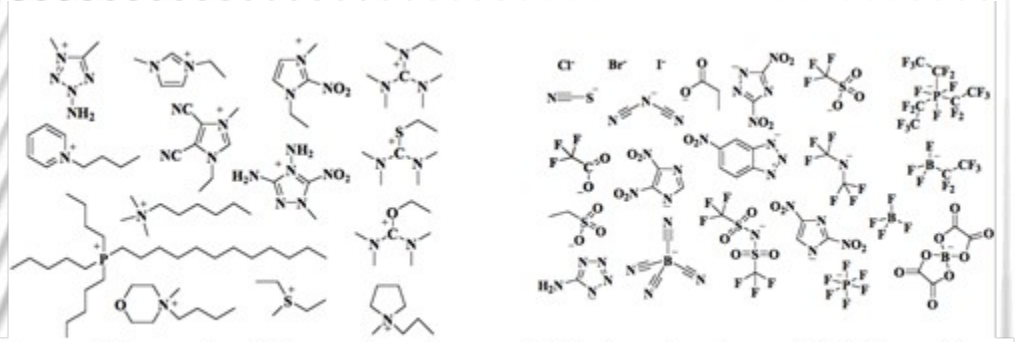


Figure 1: Examples of 14 organic cations and 25 anions leading to 350 different ILs.

Ionic Liquids

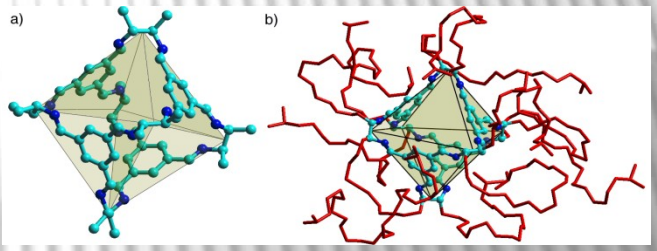


Figure 2: A typical molecular cage with alkylated chains

Porous liquids

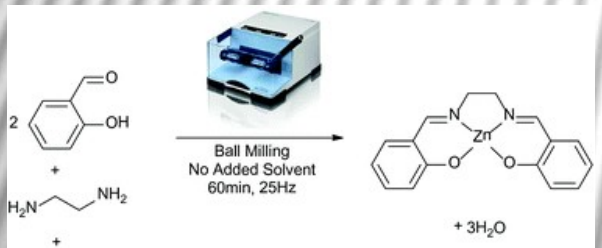
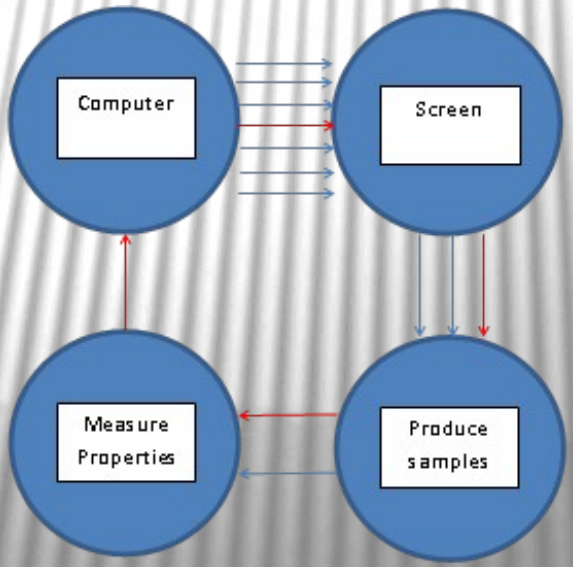
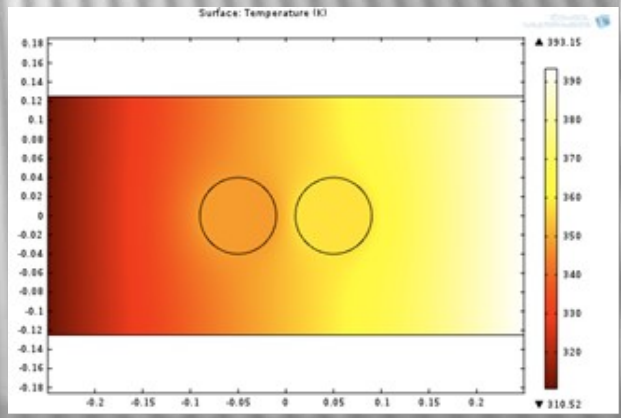


Figure 6: Schematic view of the processes occurring in a ball mill

Mechanochemistry





Heat Storage