



E-MRS 2011 Spring Meeting

Bilateral Energy Conference
Acropolis Congress Center
Nice, France

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ICAM



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Spring 11 C: Size-dependent properties of nanomaterials

Nanomaterials are the focus of numerous studies due to their novel and appealing properties strikingly different from those pertaining to their coarse-grained counterparts. This symposium addresses the recent unexpected observations and interesting predictions regarding the size-dependent physical and chemical properties of nanomaterials.

Scope:

This symposium brings the experts investigating the size-dependent properties of nanomaterials together and creates a platform to present and share their most recent results, experiences and ideas. The studies on different materials (e.g. metals and ceramics) employing various approaches (e.g. computer simulation and dedicated characterization methods) provide a better understanding of the general mechanisms governing the deviations of the properties of nanomaterials from the ones pertaining to coarse-grained materials. The discussions in the light of the broad perspective of the contributors are expected to provide possible explanations and/or clues regarding the yet unexplained size-dependent phenomena. The symposium will mainly cover, but will not be limited to, the following topics:

- Methods for the synthesis of nanomaterials
- Influence of size on phase stability
- Variations in mechanical, electronic, magnetic and thermal properties in the nanosize regime
- Size effects on type and concentration of lattice defects
- Deformation and thermally activated processes at nanoscale
- Novel properties obtained at interfaces
- Dedicated characterization of nanomaterials
- Designing new materials: Engineering the nanostructure

Hot topics to be covered by the symposium:

The following HOT topics will be emphasized in the symposium:

- Synthesis of nanocrystalline metals and ceramics: Bulk, powder and thin film
- New properties at interfaces
- Nanomaterials for energy technologies
- Size-dependent deformation mechanisms
- Grain boundary structure and migration kinetics
- Bio-inspired nanocomposites
- Advanced methods for the characterization of nanostructures

15:15 MODELLING THE SIZE-DEPENDENCE EFFECTS ON THE ELECTRONIC PROPERTIES OF CONJUGATED OLIGOMERS

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Resume : Conjugated oligomers are materials that have the potential to be used in organic and hybrid electronic and optoelectronic devices as an active component. However, the electronic properties responsible for their electrical and optical behaviour are size-dependent. Here we use a self-consistent quantum molecular dynamics method to study the effect of the oligomers length at nanosize regime on the ionization potential, electron affinity, charge (electrons and holes) mobility along the conjugated oligomer, electronic exciting energies and relaxed exciton energies. Our results show a large variation in these properties with the length of the conjugated oligomer, the effect being more pronounced for oligomers with a conjugation length lower than 6 monomers.

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