Comitato Scientifico
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VENUE

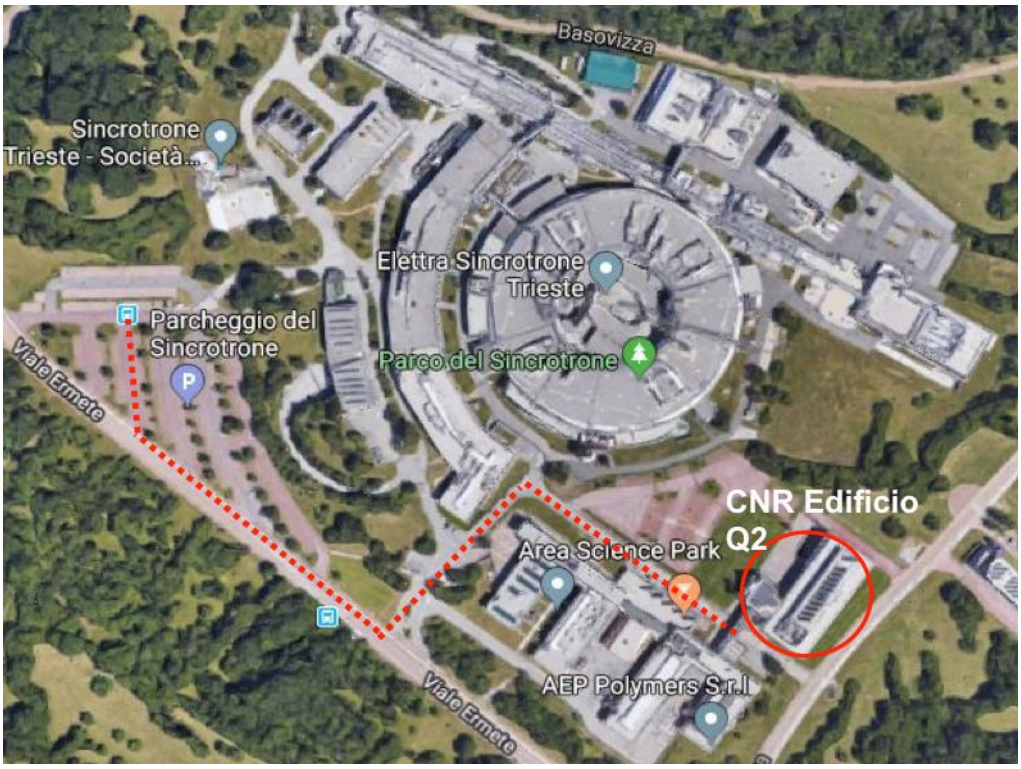
Il workshop si terrà all'interno dell'edificio Q2 nella Sala seminari "Massimo Sancrotti" al primo piano.

La poster session ed il coffe break saranno allestiti nell'edificio Q2 al piano terra.

Nella mappa è indicato il percorso per raggiungere l'edificio Q2 dalla fermata dell'autobus.

Ulteriori informazioni si possono trovare nella pagina web del workshop:

http://www.elettra.eu/Conferences/2020/MOST/



PROGRAM

Monday, 20 January 2020

Arrival and registration

12:30 Arrival and registration

Section A

Chair: M. Coreno

14:15 *L. Avaldi*
Opening Speech

14:20 *A. Franciosi*
Welcome Speech

14:35 *B. Diviacco*
Status of the Undulator Development

14:50 *M.N. Piancastelli*
Perspectives for AMO research in the soft x-ray range

15:20 *P. Decleva*
A dialogue between theory and experiment

15:50 *L. Poletto*
Innovative instrumentation for ultrafast XUV photon handling: the role of the MOST beamline

Coffee Break & Poster Session

16:10
17:10 Coffee Break & Poster Session

Section B

Chair: A. Ciavardini

17:10 *F. Fiore*
Laboratory Measurements of Wavelength and Cross-Sections of Atomic Inner-Shell Transitions from Abundant Elements in Astrophysics

17:30 *P. Bolognesi*
Radiosensitisers and radiation damage

17:50 *A. Maris*
Studying isomerism through in silico, XPS and microwave experiments

18:10 *L. Aversa*
Organic molecules seeded in supersonic molecular beams: a different approach to gas phase analysis and deposition/adsorption on surfaces.

18:30 *A. Cartoni*
Ion-Molecule Reaction Dynamics

20:00 Social Dinner at "Il Tiglio"

Tuesday, 21 January 2020

Section C

Chair: K. C. Prince

09:00 *S. Stranges*
Upgrade of current experimental methods to benefit from the new Elettra 2.0 photon source in multi-particle detection spectroscopies, and in studying highly reactive materials

09:20 *S. Falcinelli*
Coulomb explosion dissociation processes of simple organic molecules by ionizing radiations in space

09:40 *P. Piseri*
Developing core-level spectroscopy methods on free-nanoparticles: multiple coincidence experiments on clusters from transition metals in a molecular beam

10:00 *A.C. Marcelli*
Characterization of VOCS by spectroscopic techniques

Coffee Break & Poster Session

10:20
11:20 Coffee Break & Poster Session

Section D

Chair: S. Turchini

11:20 *F. Morini*
Molecular Dynamics and Electron Momentum Spectroscopy

11:40 *S. Coriani*
Ab initio coupled cluster methods for local, ultrafast and chiral spectroscopies

12:00 *M. Stener*
Origin of Circular Dichroism in noble metal clusters by TDDFT

12:20
Discussion and closing remarks
13:20

Radiosensitisers and radiation damage

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Radiosensitisers for enhancing the therapeutic efficacy of cancer treatment continue to be actively investigated, both at the macroscopic level of cells and tissues [1] and at the fundamental level of model systems, considered as isolated species in the gas phase [2,3]. After several years of intensive work from the international community, strengths and limits of these two approaches have become clear. The first, based on 'trial and error', can provide realistic responses, while the second, which allows a complete characterization of processes and mechanisms, needs validation in real biological samples. Now it is time to bridge the gap between these two complementary approaches. This implies to apply highly advanced physical chemical methods to the study of both more realistic and complex systems in the gas phase and of species and processes in realistic environment.
In the context of radiotherapy, metallic nanoparticles (NPs) like AuNP, AgNP, PtNP and GdNP have attracted increasing interest for their capacity to enhance radiation damage [4]. The primary interaction with the therapeutic beam leads to the deposition of several tens of keV in the tumor area (K, L and M ionization of the metal atoms). This energy is subsequently redistributed in the surrounding medium via de-excitation of the NPs. Cascade photon and Auger electron emission may ionize surrounding biomolecules as well as neighboring NPs, triggering new processes at lower excitation energies. Examples of these processes triggered by the secondary particles with energy transfer from few eV to few hundreds of eV to NPs are plasmon resonant excitation and metal atom d-shell ionization/excitation. Even though each single event involves a limited energy transfer, their high cross section and large number, due to the amount of secondary particles produced by the primary ionisations, make them very effective among the radiosensitising mechanisms [5]. In addition, they trigger additional damaging processes by water ionization and OH radical formation as well as by dissociative electron attachment, depending on the kinetic energy of the emitted electrons.
In this context which is currently mostly covered by theoretical simulations, both the i) absorption cross section from plasmon excitation (laser or electron collision in laboratory based experiments) to d-shell metal excitation/ionization (tunable synchrotron radiation) and ii) their secondary electron emission need to be studied in NPs with different metals and of different size. Moreover, the effects of the NP coatings and functionalizations have to be experimentally investigated.
The challenges are on one side the production of complex species like NP and large biomolecular clusters and on the other the availability of a tunable and intense VUV and soft-X ray source combined with high efficient instruments which overcome the low density of the target beam and allow to detect electrons in conjunction with other ionisation/decay products. The technical specs of MOST and the end stations that can be designed [6] may offer the possibility to tackle successfully these challenges.

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References:
1 Z. Kuncic and S. Lacombe, Phys. Med. Biol. 63, 02TR01 (2018)
2 R. Meißner et al., Nature Communications 10, 2388 (2019)
3 P. Bolognesi et al., Front. Chem. 7, 151(2019); J. Chiarinelli et al. Front. Chem. 7, 329 (2019) 4 S.J. McMahon et al., Nanoscale, 8, 581 (2016)
5 A.V. Verkhovtsev et al. PRL 114, 063401 (2015)
6 L.S. Wang, J. Chem. Phys. 143, 040901 (2015)