
Contribution ID: **32** Type: **not specified**

# The role of metals in the Alzheimer disease. Experiments and ab initio simulations

*Wednesday, 9 December 2015 17:00 (30 minutes)*

The simultaneous development of new algorithms and powerful computers together with more and more advanced experimental techniques, is opening a new era where numerical and experimental approaches will be synergistically employed to make us understanding phenomena until recently unattainable.
I will highlight the importance of the complementary use of experiments and numerical approaches in an especially relevant scientific problem that has to do with the role played by metals in the development of Amyloid diseases (also called Protein Conformational Diseases (PCD's)) to which the Alzheimer disease (AD) in particular also belong.
The hallmark of PCD's is the misfolding and subsequent aggregation of a certain protein, that in AD is actually a short amino acidic sequence (a peptide) called the A-beta peptide, that is known to be able to bind metal ions, in particular Cu(II) and Zn(II). The role played by metal ions in the development of the pathology is a necessary piece of information to find successful strategies against AD.
Among the many experimental techniques that are at our disposal to attack the problem of clarifing the biochemical basis of protein misfolding and aggregation, X-ray Absorption Spectroscopy, appropriately complemented by numerical (classical and ab initio) simulations, represents a very promising approach.
I will present a few examples where synergistically experiments and simulations have been successfully employed.

**Primary author:** Prof. MORANTE, silvia (department of physics University of Rome Tor Vergata)

**Co-authors:** Prof. ROSSI, Giancarlo (departmente of physics University of Rome Tor Vergata); Dr STELLATO, francesco (INFN Sez Tor Vergata Roma); Dr MINICOZZI, velia (deprtment of physics university of rome tor vergata)

**Presenter:** Prof. MORANTE, silvia (department of physics University of Rome Tor Vergata)

**Session Classification:** Session 2