Solvay Colloquium

Professor Pekka Pyykkö

(University of Helsinki, Finland)

SOME HIGHLIGHTS IN RELATIVISTIC QUANTUM CHEMISTRY OF HEAVY ELEMENTS

The Relativistic Theory of Atoms and Molecules (RTAM) has become a vast field of about 17000 papers, see the bibliography [1], rtam.csc.fi. The fundamentals at Dirac-Fock-Breit level, including simple treatments of the Lamb shift, seem to be under control [2]. Numerous reviews exist on these effects in Inorganic Chemistry [3,4] and qualitative estimates on them have entered most textbooks of Inorganic Chemistry.

The main message is that many of the differences between the Periods 5 and 6 can be explained by relativistic effects. Some examples are the difference between silver and gold, between cadmium and mercury, or between tin and lead. Most of the voltage of the lead battery is due to relativity [4]. Some further issues in simple bonding theory are the covalent radii [5], or the concept of oxidation states [6].

References:
[1] P. Pyykkö, J. Comp. Chem. 34 (2013) 2667
[2] P. Pyykkö, Chem. Rev. 112 (2012) 371
[3] P. Pyykkö, Chem. Rev. 88 (1988) 563
[4] P. Pyykkö, Ann. Rev. Phys. Chem. 63 (2012) 45
[5] P. Pyykkö, J. Phys. Chem. A 119 (2014) 2326
[6] P. Pyykkö, W.-H. Xu, Chem. Eur. J. 21 (2015)

Tuesday 17 November 2015 at 4.00 P.M.

COFFEE AND TEA WILL BE SERVED AT 3.45 P.M. IN FRONT OF THE SOLVAY ROOM

SOLVAY ROOM

Building N.O. - 5th Floor
Université Libre de Bruxelles
Campus Plaine - Boulevard du Triomphe
Access 2- 1050 Brussels

www.solvayinstitutes.be