# The 32-Electron Principle: A New Magic Number

**J.-P. Dognon**

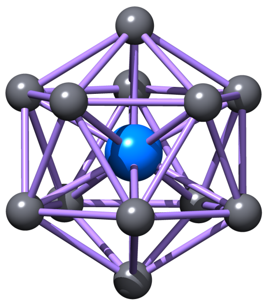
*CEA/Saclay, DRF/IRAMIS/NIMBE, UMR 3685 CEA/CNRS NIMBE*

*Laboratoire Structure et Dynamique par Résonance Magnétique (LSDRM)*

*91191 Gif-sur-Yvette, France*

*e-mail: jean-pierre.dognon@cea.fr*

The Lewis octets and the Langmuir 18-electron (18e) rule are well-known principles in inorganic chemistry [1]. The key point is that, up to 18e, s-, p-, and d-like orbitals of the total system are fully occupied. The next step would be adding an f-like shell with 14 further electrons, giving a total of 32 electrons. If any f-contributions are desired at a central atom, an actinide is required. We first predicted from quantum chemical calculations that this could, indeed, be achieved in the isoelectronic series of icosahedral Pu@$Pb_{12}$ [2]. Other cases, identified by us, are the isoelectronic series of U@$C_{28}$ [3] and the case Pu@$Sn_{12}$ [4]. Before being able to claim the 32-electron rule as a chemical principle, it is desirable to have further examples. A new case reported is based on an actinide (U, Np, Pu, Am and Cm), doping a cage of silicon, $Si_{20}$ [5]. The stability of the charged systems is energetically favored by chemical bonding between the central atom and the Si cage supported by energy partitioning and topological analyses [6,7]. One neutral 32-electron system is also presented by adding two electron-donor lanthanide atoms on the pentagonal faces of the $Si_{20}$ cage. Combined with appropriate hexohedral electron donor atoms, the existence of this very stable silicon-based family suggests that it should be possible to create Si-based clusters containing early actinides, and to assemble further structures from them.



Our purpose here is to cover the recently discussed 32e compounds [8] and theoretically predicted as very stable species that should be accessible experimentally. The future will show how many 32e systems will turn up.

## References

1. P. Pyykkö, *J. Organomet. Chem.*, **2006**, *691*, 4336.
2. J.-P. Dognon, C. Clavaguéra, P. Pyykkö, *Angew. Chem. Int. Ed.*, **2007**, *46*, 1427.
3. J.-P. Dognon, C. Clavaguéra, P. Pyykkö, *J. Am. Chem. Soc.*, **2009**, *131*, 238.
4. J.-P. Dognon, C. Clavaguéra, P. Pyykkö, *Compt. Rend. Chimie*, **2010**, *13*, 884.
5. J.-P. Dognon, C. Clavaguéra, P. Pyykkö, *Chem. Sci.*, **2012**, *3*, 2843.
6. J.-P. Dognon, *Coord. Chem. Rev.*, **2014**, *266–267*, 110.
7. J.-P. Dognon, *Coord. Chem. Rev.*, **2017**, *150-162, 344.*
8. P. Pyykkö, C. Clavaguéra, J.-P. Dognon, *in Computational Methods in Lanthanide and Actinide Chemistry*, ed. M. Dolg, Wiley., **2015**, 401