NOVEL SANDWICH-LIKE COMPLEXES BASED ON INORGANIC AROMATIC COMPOUNDS

Jose M. Mercero, Jon M. Matxain and Jesus M. Ugalde
Kimika Fakultatea, Euskal Herriko Unibertsitatea,
P.K. 1072, 20080 Donostia

jm.mercero@ehu.es

We report novel sandwich-like structures formed between the aromatic squares Al_4^{2-} [1] and N_4^{2-} [2]. This structures have two aromatic squares (2- charged each) trapping a positively charged TM. The predicted sandwiches for the Al square are formed with Ti, V and Cr, the three sandwiches have the same number of electrons[3]. For N square, also sandwiches for Fe, Co and Ni have been found[4]. The changed suffered by the squares after forming the sandwich is very small, and aromatic properties are manteined in most of the cases. Some of these sandwiches have 2- charge, and exhibit negative electron detachment energies. The use of alkali metals to stabilize them is also analized. Finally, the possibility of the Ti and Fe, N sandwiches to oligomerize is disccussed. We have not been able to found analogous structures for Al squares yet.

References:

[1] Li, X.; Kuznetsov, A. E.; Zhang, H. F.; Boldyrev, A. I.; Wang, L.-S. *Science*, **291**, (2001), 859.
[2] Li Q. S.; Cheng L. P. *J. Phys. Chem*. **107** (2003) 2882.
[3] Mercero, J. M. and Ugalde J. M. *J. Am. Chem. Soc,* **126** (2004), 3380.
[4] Mercero, J. M.; Matxain J. M and Ugalde J. M. *Angew. Chem., Int. Ed. In Press*

Figures:

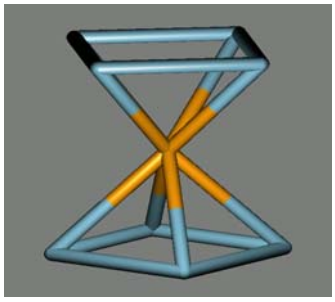

Figure 1: AlXAl ground state Sandwich for X=Ti,V, and Cr (ch=-2,-1, 0).

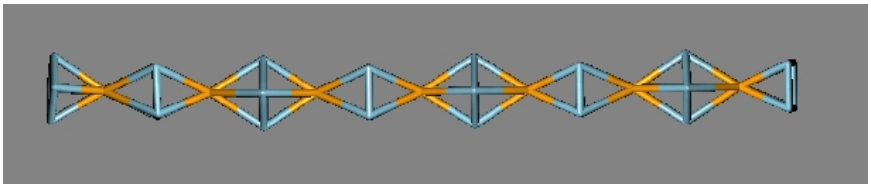

Figure 2: Fe, N Fe-N4 sandwich oligomer.