MOLECULAR ELECTRIDES AND METALLAELECTRIDES

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Electrides are unique ionic compounds where the anionic part is constituted only by isolated electrons. These new type of compounds were postulated and synthesized first by Dye.[1] They have interesting physicochemical properties that make them suitable for certain technological applications. Thus far, only *solid-state* electrides have been reported. Electrides were shown to exhibit large non-linear optical properties (NLOP),[2] non-nuclear attractors (NNA) of the electron density, and electron localization function (ELF) basins. However, several molecules show some of these properties without the presence of an isolated electron. Therefore, none of these properties alone are sufficient to characterize electrides. In this work, we provide an unambiguous computational means to distinguish *molecular* electrides from similar species.[3] We analyze seven species that were previously considered molecular electrides on the basis of large NLOPs and frontier orbitals with large density values in the position where one would expect the isolated electron of the electride. We show that some of them are actually not electrides.[3] Finally, we present two examples (O_h Li_6^+ with S=3/2 and Be_6 with S=2) of a new type of *molecular* electrides that we name metallaelectrides. They are characterized by having more NNA than atoms and all (or most of) the valence electron density located in the NNA regions. These species can be considered molecular models for the study of the metallic bond.[4] We will show that Li_n clusters (n = 2–8) having different spins show a smooth transition from the electride to the metallaelectride character.

References
1) J. L. Dye, *Acc. Chem. Res.* **2009**, *42*, 1564.
2) M. Garcia-Borràs, M. Solà, J. M. Luis and B. Kirtman, *J. Chem. Theory Comput.* **2011**, *8*, 2688.
3) V. Postils, M. Garcia-Borràs, M. Solà, J. M. Luis and E. Matito, *Chem. Commun.* **2015,** *51*, 4865.
4) O. El-Bakouri, V. Postils, M. Garcia-Borràs, M. Duran, J. M. Luis, E. Matito, S. Calvello, A. Soncini, F. Feixas and M. Solà, to be submitted.