

Excess Electron Compounds Simultaneously Containing Electride and Alkalide Characteristics: Unique Electronic Structures and Remarkably Large Nonlinear Optical Responses

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Abstract

A intriguing type of excess electron compounds simultaneously containing electride and alkalide characteristics was obtained on the basis of the synthesized facially polarized molecule all-cis 1,2,3,4,5,6-hexafluorocyclohexane (1). By doping the two different faces of this Janus molecule with an alkaline earth atom and an alkali-metal atom, a series of M-1-M' (M = Be, Mg, and Ca; M' = Li, Na, and K) compounds were firstly achieved. Our calculated results show that, different from Be and Mg, one 4s electron of Ca can be transferred to the upper alkali metal atoms forming an alkali metal anion while the remaining 4s electron was push away from Ca⁺ yielding an electron anion by the instinctive facial polarization of 1 or with the assist of oriented external electric fields (OEEFs). Owing to the existence of two loosely bound excess electrons in the resulting Ca⁺-1-M' (M' = Li, Na, and K), these novel compounds exhibit extremely large first hyperpolarizabilities (β_0) of 9.94×10^5 - 1.81×10^6 au. Thus, we hope that this work could provide the first members with both of electride and alkalide characteristics to further enrich the family of excess electron compounds.

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