

Supporting Information

A Simplified and Facile Preparation Method for $[\text{Ca}_{24}\text{Al}_{28}\text{O}_{64}]^{4+}(\text{e}^{-})_4$ Electride

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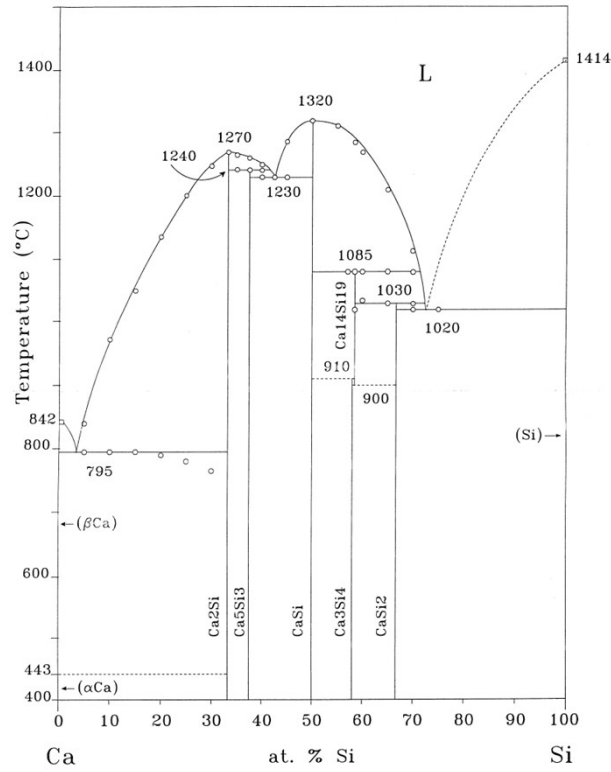


Figure S1. The binary alloy phase diagram of Ca and Si.^[1]

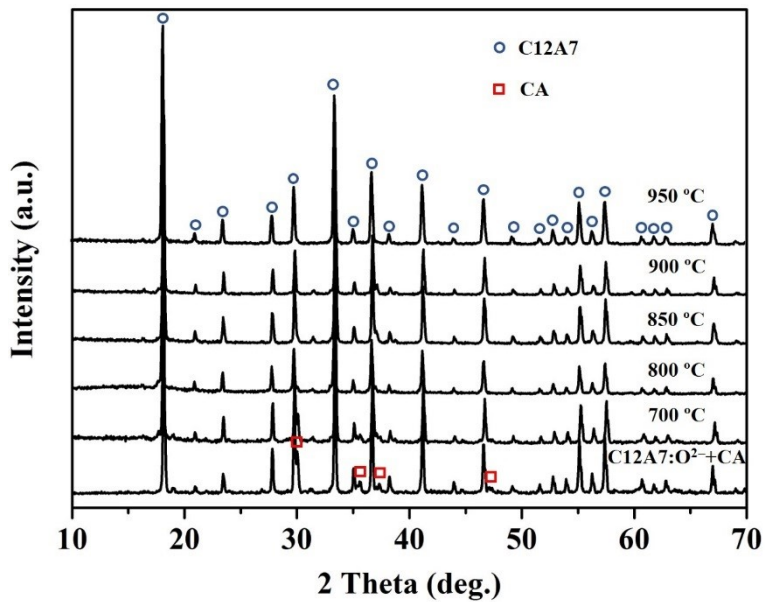


Figure S2. Powder XRD patterns of C12A7:O²⁻+CA and CaH₂ at different calcination temperature. All obtained powders were washed with a solution of 0.1 M NH₄Cl in methanol.

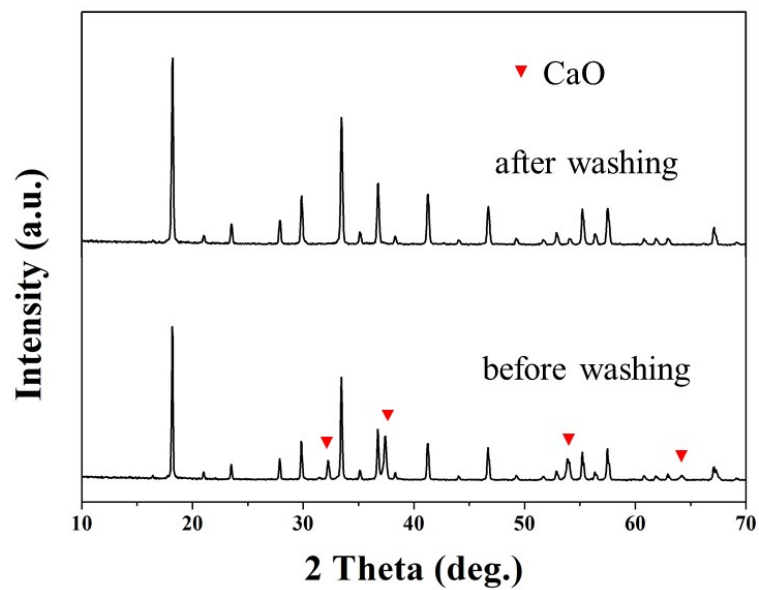


Figure S3. Powder XRD patterns of before and after washing of C12A7:O²⁻+CA and CaH₂ at 950 °C.

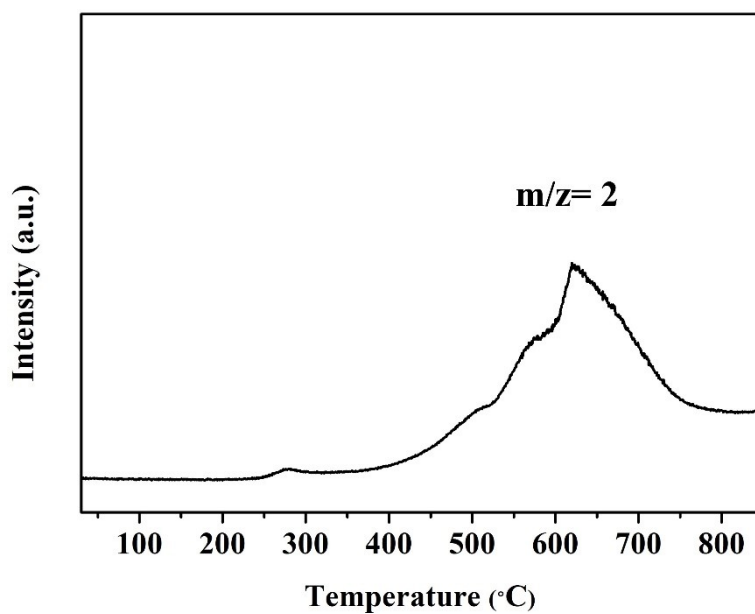


Figure S4. TPD profile of C12A7:e⁻ powder.

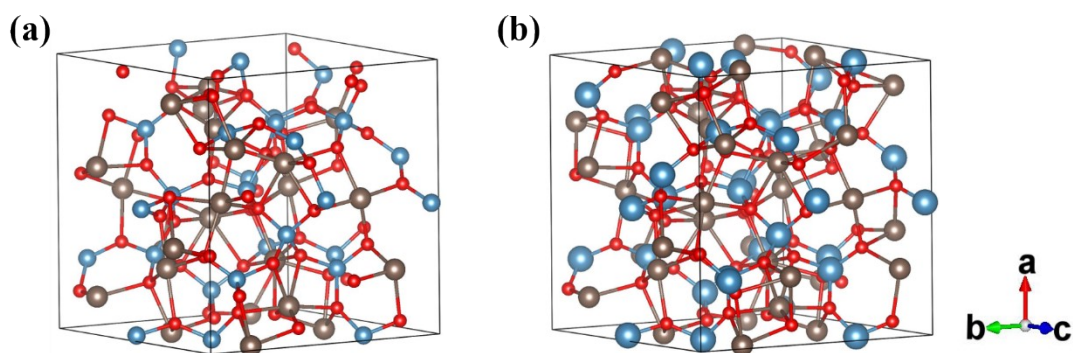


Figure S5. The optimized structure models of C12A7:O^{2-} and C12A7:e^- .

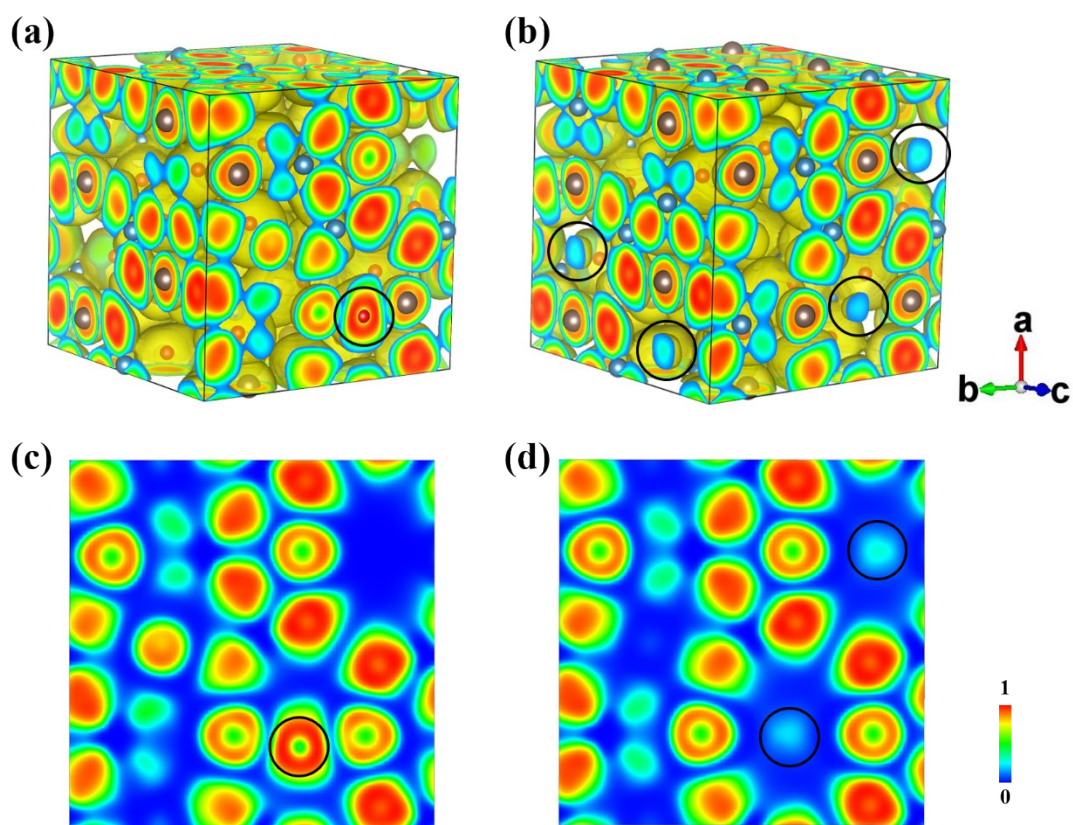


Figure S6. Isosurface of electron localization function (ELF) with the value of 0.1 for C12A7:O^{2-} (a) and C12A7:e^- (b). ELF map in the (001) plane of C12A7:O^{2-} (c) and C12A7:e^- (d). The O (cage) and interstitial electrons are respectively encircled by black circles.

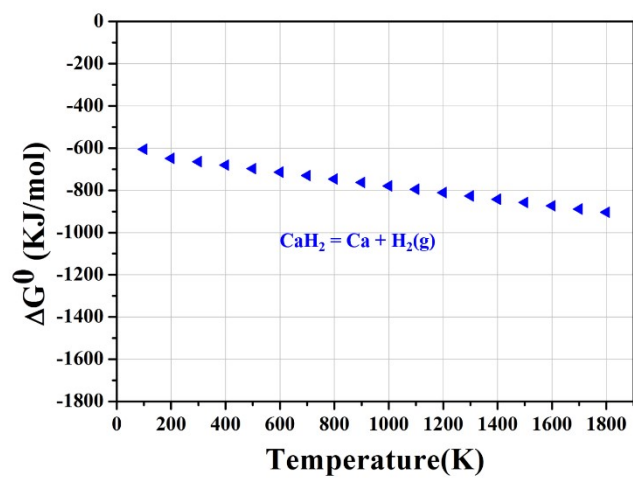


Figure S7. Thermodynamics analysis of the CaH_2 decomposition. It is indicated that CaH_2 decomposition is intensively exothermic process.

REFERENCES

- [1] P. Manfrinetti, M. L. Fornasini, A. Palenzona. *Intermetallics*, 2000, **8**, 223.