

ポスター | R2：結晶構造・結晶化学・物性・結晶成長・応用鉱物

2026年9月25日(金) 12:30 ~ 14:00 | ポスター (336, 340, 341号室)

R2：結晶構造・結晶化学・物性・結晶成長・応用鉱物

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[R2P-03] First-Principles Study of Iron Substitution Preference and Optimal Doping Concentration in Jonlarsenite (γ -Al₄Cu₉)三河内 岳³ (1. Macau Univ. Sci. Tech., Fac. Innov. Eng., 2. Macau Univ. Sci. Tech., State Key Lab. Lunar Planet. Sci., 3. Univ. of Tokyo, Univ. Museum)

キーワード：First-principles study、Iron substitution preference、Jonlarsenite

Jonlarsenite (IMA 2024-078a) is a newly identified extraterrestrial γ -Al₄Cu₉ intermetallic phase found in a micrometeorite and named after Norwegian mineral collector Jon Larsen [1]. Jonlarsenite occurs as very small particles (up to ca. 2 microns) and crystallizes in a cubic lattice, space group P-43m. Its structure was determined by high-resolution transmission electron microscopy (TEM) and complementary microanalytical techniques [1]. The calculated density is about 6.98 g cm⁻³. Jonlarsenite represents a confirmed natural example of the γ -Al₄Cu₉ intermetallic phase, a composition that is rarely observed in nature. Its occurrence in a meteoritic particle provides evidence for high-temperature formation and rapid cooling or shock-related processes in the early solar system or parent body environments. The discovery helps constrain phase equilibria and thermal histories of Al-Cu bearing phases in extraterrestrial materials and offers a useful marker for interpreting high-temperature events in meteorites.

Due to interest in iron (Fe) doping in Al-Cu compounds, this work investigates the Fe substitution preference and optimal doping concentration in jonlarsenite using first-principles density functional theory (DFT). We evaluated the formation energies of different Fe substitution ratios in a γ -Al₄Cu₉ unit cell (52 atoms in total) using CASTEP in Materials Studio. Among all the calculated models (listed in Table 1), in the models where Fe substitutes Cu sites (models a-f), the formation energy reaches a distinct minimum at the higher Fe substitution concentration (Al₁₆Fe₁₆Cu₂₀), particularly in model d (Fig. 1). In contrast, lower Fe concentrations result in higher formation energies, such as -9.5183 eV at a substitution rate of 16.7% (model b) and -8.5218 eV at 33.3% (model c). Furthermore, Fe substitution at Al sites (model g) leads to a significantly higher formation energy of -5.1033 eV, confirming that Fe substitution on Al sites is thermodynamically unfavorable. The large energy difference between model d and its isomers (models e and f) indicates that the substitution concentration is not the sole factor determining the stability of the system. The ordering behavior of the substitution sites in the lattice also significantly affects the formation energy. In summary, Fe preferentially substitutes at Cu sites, and the synergistic effect of high Fe doping concentration (44.4%) combined with an ordered atomic arrangement enables the Al-Cu intermetallic compound to achieve thermodynamic stability.

Reference: [1] Bindi L. et al. (2025) *Eur. Jour. Mineral.*, 37, 783-791.

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Table 1. The models and formation energies E_f of Fe-doped γ - Al_4Cu_9 .

Model	Chemical formula	Fe occupancy	E_f (eV)
a	$\text{Al}_{16}\text{Fe}_6\text{Cu}_{30}$	on Cu sites (16.7% replacement)	-9.5179
b	$\text{Al}_{16}\text{Fe}_6\text{Cu}_{30}$	on Cu sites (16.7% replacement)	-9.5183
c	$\text{Al}_{16}\text{Fe}_{12}\text{Cu}_{24}$	on Cu sites (33.3% replacement)	-8.5218
d	$\text{Al}_{16}\text{Fe}_{16}\text{Cu}_{20}$	on Cu sites (44.4% replacement)	-10.6308
e	$\text{Al}_{16}\text{Fe}_{16}\text{Cu}_{20}$	on Cu sites (44.4% replacement)	-6.1335
f	$\text{Al}_{16}\text{Fe}_{16}\text{Cu}_{20}$	on Cu sites (44.4% replacement)	-7.1024
g	$\text{Al}_{12}\text{Fe}_4\text{Cu}_{36}$	on Al sites (25% replacement)	-5.1033

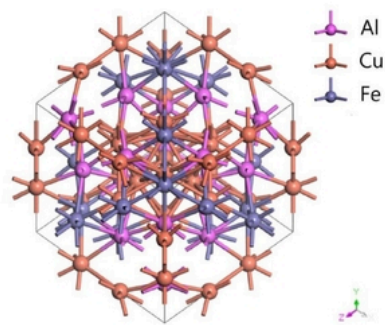


Fig. 1. The optimal crystal structure of Fe-doped γ - Al_4Cu_9 (Model d, $\text{Al}_{16}\text{Fe}_{16}\text{Cu}_{20}$). Colors: pink, orange, and purple spheres represent Al, Cu, and Fe atoms, respectively.