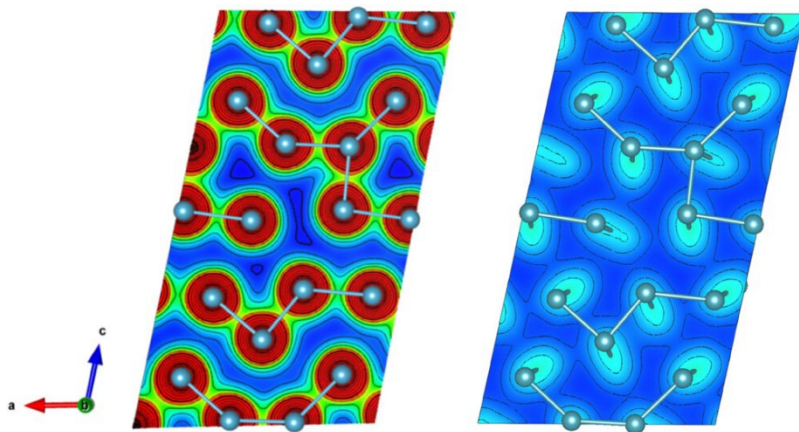


# Confirmation of Covalent Bonding in $\alpha$ -Pu



**The charge structure of  $\alpha$ -Pu.** (Left) The charge density in the atomic plane shows distinct signatures of bonding exist between neighboring atoms at short bond lengths. (Right) The charge density on the interatomic plane shows less charge between neighboring atoms.

A. R. Muñoz, M. S. Cook, D. C. Arellano, A. M. Abeykoon, J. N. Mitchell, S. C. Hernandez, E. D. Bauer, C. A. Mizzi, B. Maiorov, N. Harrison, W. A. Phelan, Experimental and Theoretical Confirmation of Covalent Bonding in  $\alpha$ -Pu. *Adv. Funct. Mater.* 2025, 2501798. <https://doi.org/10.1002/adfm.202501798>

Work was performed in part at NSLS-II

## Scientific Achievement

Scientists uncover joint experimental and theoretical evidence of covalent bonding in  $\alpha$ -plutonium ( $\alpha$ -Pu) for the first time.

## Significance and Impact

Atomistically understanding how different types of bonding influence Pu allotrope behaviors could reshape how these materials are used for nuclear energy applications, like batteries and reactors.

## Research Details

- Density functional theory and pair distribution functions obtained from X-ray diffraction was used to study the bonding behavior in  $\alpha$ -Pu.
- First experimental and theoretical description of local bonding behavior for  $\alpha$ -Pu revealed covalent bonds.
- Short bond distances have a directional, covalent-like nature, while longer bonds have a more metallic character.