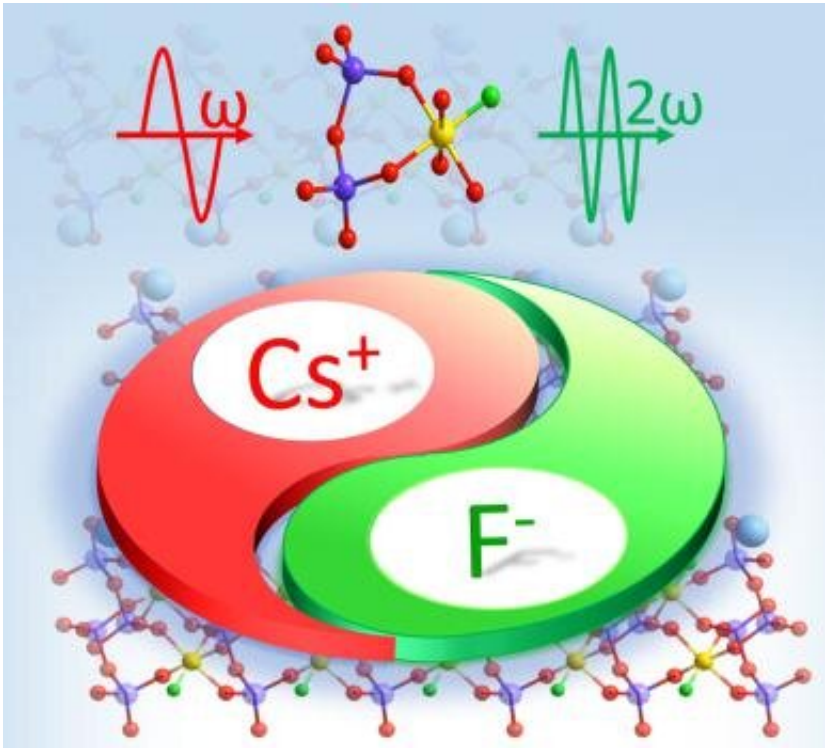
Research uncovers the first non-centrosymmetric fluorooxosilicophosphate with Si-F bonds

April 27 2020, by Liu Jia



Schematic illustration of the research. Credit: Prof. LUO's group

Deep-ultraviolet (UV) nonlinear optical materials play a vital role in a variety of high-tech scientific instruments. Traditionally, the sources of these materials were usually limited to π-conjugated systems such as borates and carbonates, while the non-π-conjugated system such as

phosphates and silicates is relatively unexplored.

In a study published in *J. Am. Chem. Soc.*, a research group led by Prof. Luo Junhua and Prof. Zhao Sangen from Fujian Institute of Research on the Structure of Matter (FJIRSM) of Chinese Academy of Sciences, reported a new non-π-conjugated nonlinear optical fluorooxosilicophosphate $CsSiP_2O_7F$, which is the first non-centrosymmetric fluorooxosilicophosphate with Si-F bonds.

The researchers found that the introduction of the element cesium with the least electronegative property and the element fluorine with the largest electronegative helps to form the non-centrosymmetric structure of $CsSiP_2O_7F$. In this structure, the element cesium forms locally asymmetric CsO_5F_2 polyhedra and element fluorine forms SiO5F species to lower the local symmetry of $SiP_2O_{10}F$ moiety.

The second harmonic generation (SHG) intensity of powder $CsSiP_2O_7F$ sample is approximately 0.7 times that of KH_2PO_4 and shows phase-matching behavior. According to the first-principles calculations, the SHG response mainly results from the unprecedented $SiP_2O_{10}F$ moiety. As a result, the $SiP_2O_{10}F$ moiety in this structure is a new type of nonlinear optical active gene.

In addition, relevant experimental and calculated results indicated that $CsSiP_2O_7F$ is deep-UV transparent, and both cesium and fluorine favor the deep-UV transparency of $CsSiP_2O_7F$.

This study provides a new source for deep-UV nonlinear optical materials, and insight into how to obtain non-centrosymmetric structures that are indispensible to functional materials on nonlinear optics, piezoelectricity, ferroelectric, pyroelectricity, etc.

More information: Qingran Ding et al. Designing a Deep-UV

Nonlinear Optical Fluorooxosilicophosphate, *Journal of the American Chemical Society* (2020). DOI: 10.1021/jacs.0c00060