Novel partial isovalent anion substitution induction strategy to design infrared nonlinear optical materials

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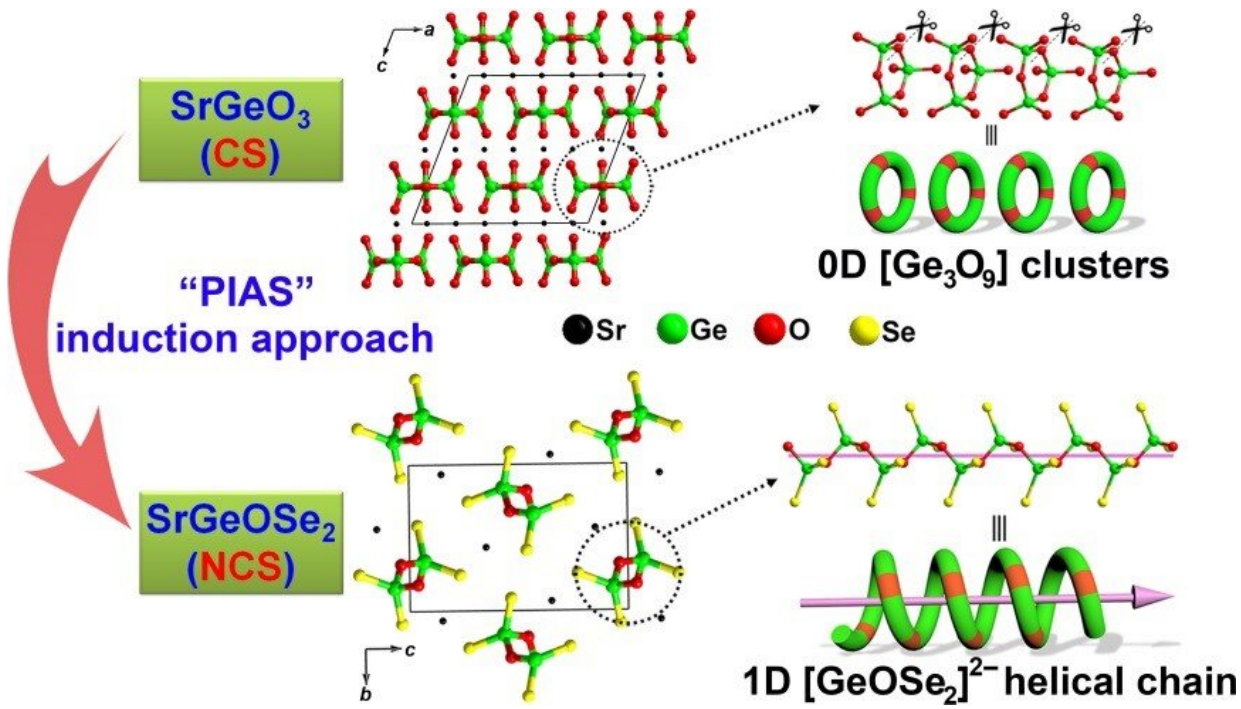

Structural transformation from CS compound SrGeO3 to the NCS SrGeOSe2. Credit: Prof. ZHU's Group

Infrared nonlinear optical (IR–NLO) materials are crucial for a broad range of applications, such as signal communication, microscopy and data processing. Yet, the challenge is how to obtain a strictly structural

non-centrosymmetric (NCS) compound, which is the primary requirement for the IR–NLO materials.

In a study published in *Chemistry of Materials*, the research team led by Prof. Zhu Qilong and Prof. Lin Hua from Fujian Institute of Research on the Structure of Matter (FJIRSM) of the Chinese Academy of Sciences proposed a partial isovalent anion substitution (PIAS) strategy to design and synthesize a novel IR–NLO material $SrGeOSe_2$.

The researchers have, for the first time, reported the structural transformation from centrosymmetric (CS) compound $SrGeO_3$ to NCS $SrGeOSe_2$ through a generic and effective PIAS strategy.

They found that $SrGeOSe_2$ exhibits the desired balance between a strong powder second harmonic generation efficiency (SHG = 1.3 × benchmark $AgGaS_2$) and a large laser-induced-damage threshold (LIDT = 36 × benchmark $AgGaS_2$).

Theoretical calculations indicated that the large second-harmonic generation (SHG) efficiency mainly originates from the cooperative effects of 1-D heteroligand $[GeO_2Se_2]$ asymmetric building units.

This study provides a powerful way to rationally induce the symmetry breaking and enhance the local dipole moments of the active units.

More information: Mao-Yin Ran et al. Partial Isovalent Anion Substitution to Access Remarkable Second-Harmonic Generation Response: A Generic and Effective Strategy for Design of Infrared Nonlinear Optical Materials, *Chemistry of Materials* (2020). DOI: 10.1021/acs.chemmater.0c02011