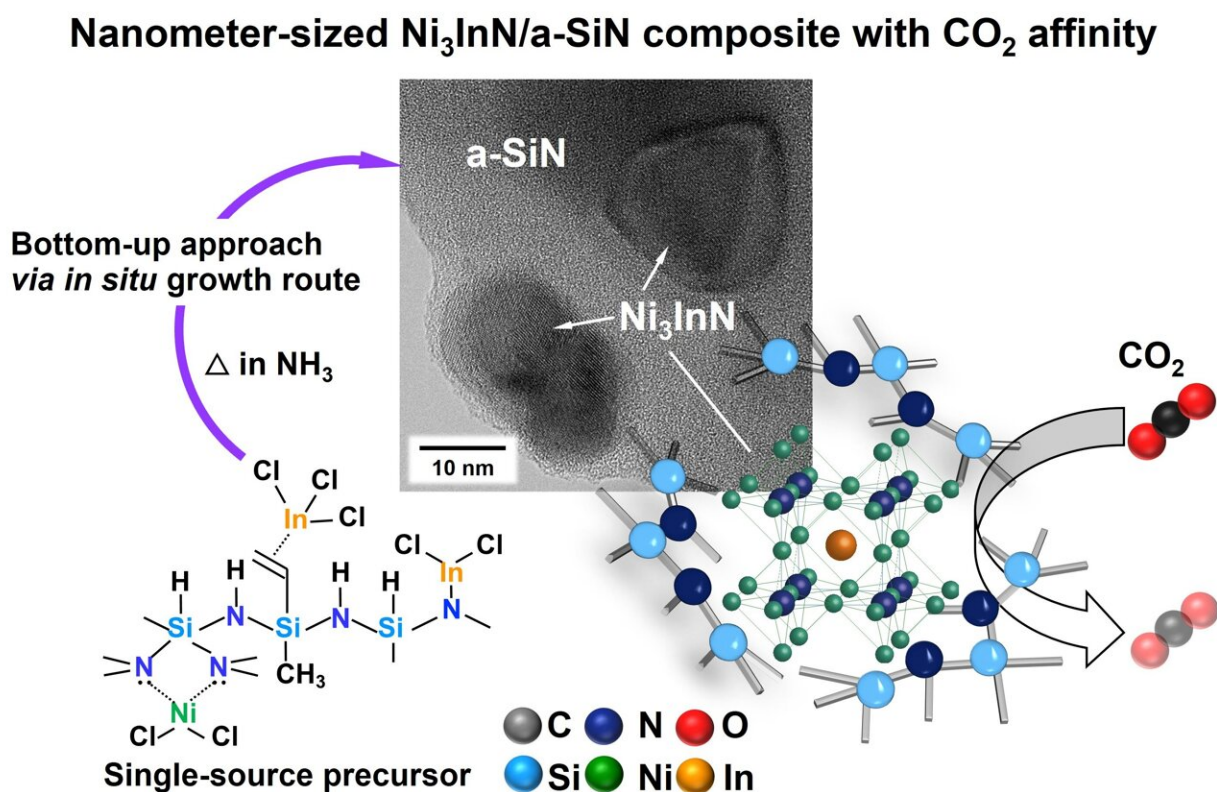


# Unlocking the potential of anti-perovskites through a convenient one-step synthesis route

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This illustration depicts a novel bottom-up approach developed to synthesize a nanometer-sized Ni<sub>3</sub>InN anti-perovskite/amorphous silicon nitride (a-SiN) nanocomposite via an *in situ* growth route, as well as its unique CO<sub>2</sub> adsorption–desorption properties as a potential small-molecule activation catalyst. Credit: Yuji Iwamoto, Nagoya Institute of Technology

Although perovskites have attracted a lot of attention lately, anti-perovskites hold just as much potential as functional materials. Bearing a similar crystal structure to perovskites but with an inverted electrical configuration, anti-perovskites exhibit peculiar properties that could be exploited, including negative thermal expansion, ionic conductivity, and even superconductivity. Unfortunately, thus far, synthesizing nanosized anti-perovskites has proven difficult, which is holding back these promising materials in catalytic applications.

In a recent study [published](#) in the *Journal of Materials Chemistry A*, a research team led by Professor Yuji Iwamoto from the Department of Life Science and Applied Chemistry at Nagoya Institute of Technology, Japan, tackled the current challenges plaguing the synthesis of nitride-based anti-perovskites. They demonstrated a convenient synthesis technique to produce a nanocomposite material consisting of amorphous silicon nitride (a-SiN) ceramic with embedded nanometer-sized Ni<sub>3</sub>InN anti-perovskite crystals.

Their work was co-authored by Young International Faculty (Visiting Faculty) Shotaro Tada and Professor Ravi Kumar from the Department of Metallurgical and Materials Engineering at Indian Institute of Technology Madras (IIT Madras), India, and Director of Research Samuel Bernard from the University of Limoges, France.

The proposed synthesis method can be classified as a "Polymer-Derived Ceramics" (PDCs) route. First, polysilazane—used as a silicon nitride precursor—is chemically modified to include NiCl<sub>2</sub> and InCl<sub>3</sub> molecules. Then, through pyrolysis in an ammonia (NH<sub>3</sub>) atmosphere at a relatively low temperature of 300 °C, the modified precursor is transformed into the a-SiN matrix with embedded anti-perovskites in a single step.

"While our research team has [previously developed a synthesis route](#) for [transition metal/a-SiN nanocomposites](#) using polysilazanes modified

with transition metal chlorides, this recent study presents a novel approach adopting multiple metal species, resulting in the in situ growth of Ni<sub>3</sub>InN intermetallic nanoparticles within an amorphous matrix," says Prof. Iwamoto.

Dr. Tada elaborates, "During the initial stages of the research, we encountered difficulties in obtaining a single-phase Ni<sub>3</sub>InN compound through stoichiometric blending. Through [systematic analysis](#) using different types of polysilazanes and spectroscopic studies, we found that the presence of vinyl groups in polysilazanes weakened the interaction with InCl<sub>3</sub> due to steric hindrance, leading to enhanced migration of In sources into pre-formed Ni nanoparticles at [lower temperatures](#). We addressed this problem by adding excess InCl<sub>3</sub>, resulting in the formation of a single phase Ni<sub>3</sub>InN."

This bottom-up synthesis strategy has several strengths. First, the resulting nanocomposite material is highly microporous and contains abundant interfaces between Ni<sub>3</sub>InN and the a-SiN matrix. Thus, it enables the modification of the electronic structure of the surfaces of the anti-perovskite nanoparticles formed in situ. Additionally, as a single-step low-temperature method, it provides a straightforward route to obtain complex, highly [functional materials](#).

The researchers also showcased, as a proof of concept, the ability of the a-SiN/Ni<sub>3</sub>InN composite to adsorb and desorb CO<sub>2</sub>, which could be key to activating and transforming small molecules into value-added compounds for clean energy applications.

"This type of nanocomposite, with its diverse multi-metal composition, exhibits promising potential for heterogeneous catalyst design. By providing structural diversity and modifiability, it could facilitate the discovery of new catalytic functionalities," remarks Dr. Bernard.

The researchers hope that these exciting findings pave the way to versatile materials with sustainable applications.

**More information:** Shotaro Tada et al, An in situ growth route towards anti-perovskite Ni<sub>3</sub>InN nanoparticles embedded within amorphous silicon nitride, *Journal of Materials Chemistry A* (2023).  
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