

Case ID:M22-032P^

Published: 9/19/2022

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Sustainable Dehydrocoupling and Hydrofunctionalization Methods for Preparing Aminosilanes, Polysilazane Coatings, and Silicones

Background

Silicon nitride, silicon oxynitride, silicon carbonitride, and silicon dioxide films are used to protect the semiconducting regions of microprocessors, memory devices, and solar panels. These coatings are prepared by atomic layer deposition (ALD) or chemical vapor deposition (CVD) using aminosilanes, or by applying perhydropolysilazane solutions. Organic polysilazane solutions are similarly used to protect the metal surfaces of automobiles, aerospace equipment, and architectural materials. The current industrial method of preparing aminosilanes, perhydropolysilazane, and organic polysilazanes involves adding chlorosilanes to the corresponding amine or ammonia. This approach is effective, but inherently inefficient since a full equivalent of ammonium salt waste is generated for each Si-N bond that is formed. Purification measures associated with the removal of this waste compromise the atom-efficiency of aminosilane monomer and polymer synthesis while significantly adding to process cost.

The catalytic dehydrocoupling of amines and silanes affords products that feature Si-N bonds while avoiding the use of corrosive halosilane reagents. It offers an atom-efficient way to prepare aminosilane ALD/CVD precursors, perhydropolysilazane, and organic polysilazanes. The hydrogen generated as a byproduct may also be collected.

Invention Description

Researchers at Arizona State University have developed novel anionic ligand platforms that allow for the development of inexpensive manganese, iron, cobalt, and nickel catalysts that dehydrocouple amines and silanes to prepare value-added CVD precursors and pre-ceramic polymers under mild conditions (ambient temperature and pressure). Limited industrial attempts to perform aminosilane coupling reveal that heterogeneous precious metal catalysts are active at higher temperatures, but are considerably less effective than the base metal catalysts discovered in this invention. Precious metals including ruthenium, rhodium, and palladium are also toxic and expensive due to their low abundance within Earth's crust.

The catalysts developed in this invention have also been shown to mediate hydrofunctionalization reactions that allow for the facile reduction of carbonyl and carboxylate compounds, the synthesis of reagents for cross-coupling reactions, and the preparation of silanes and silicones by way of alkene hydrosilylation. Alkene

hydrosilylation often relies on platinum catalysts that add cost and supply chain risk to alkylsilane and silicone preparation.

Potential Applications

- Preparation of aminosilane monomers for chemical vapor deposition applications
- Atom-efficient synthesis of polysilazane and polycarbosilazane polymers for use as coatings in the semiconductor, aviation, and automotive industries
- Catalysts for alkene, alkyne, carbonyl or carboxylate hydrofunctionalization (preparing silicones without the need for platinum reagents)

Related Publication: [An aryl diimine cobalt\(i\) catalyst for carbonyl hydrosilylation - Chemical Communications \(RSC Publishing\)](#)