Exploring the versatility of silatranization: molecular engineering of silatrane coupling agents toward facile surface functionalization of nanomaterials in diverse media

Scientific goal of the project

The main objective of this project is to develop efficient surface treatment protocols for mineral nanofillers in both wet and dry environments, using *C*-substituted silatranes as next-generation coupling agents with improved solubility. To achieve this, silatrane derivatives bearing selected organofunctional groups will be equipped with appropriate hydrophobic and/or hydrophilic substituents on the silatranyl cage via chemical modification. These synthesized coupling agents will then be applied to surface treatment of mineral fillers for photocurable resins. Finally, the prepared resin mixtures will be evaluated in 3D printing applications. Through these steps, the effect of SilCA structure on the properties of the resulting composite materials—such as curing kinetics, cross-link density, and mechanical properties—can be assessed.

Research description

In this project, a range of silatrane coupling agents with tailored structures will be designed and synthesized to be compatible with photocurable resins. Next, a series of resin mixtures comprising organic resin monomers, surface-treated nanofillers, and a photoinitiating system will be prepared and their performance in additive manufacturing will be evaluated. The experimental work includes: (1) synthesis and characterization of silatrane coupling agents, (2) surface modification of inorganic nanofillers, (3) full characterization of the functionalized nanomaterials, (4) preparation of photocurable resin mixtures that polymerize via radical and/or cationic mechanismm, (5) optimization of photochemical 3D-printing parameters, and (6) determination of dynamic mechanical properties, cross-linking density and hydrolysis resistance of the 3D-printed objects.

Rationale for undertaking the research topic

Silatrane coupling agents (SilCAs) have recently emerged as promising alternatives to traditional silane coupling agents due to their significantly improved water resistance. With a reduced tendency for unwanted pre-hydrolysis, SilCAs allow the surface modification process to be controlled with far greater precision than their silane counterparts. These advantages provided particularly good application results in antimicrobial coatings, metal nanoparticle grafting, and biomolecule immobilization. However, a notable limitation of SilCAs is their relatively low solubility in various solvents compared to commercial silanes. To address this issue, functionalization of the carbon atoms in the silatranyl cage with solubilizing hydrophilic and/or hydrophobic side groups is proposed to enhance solubility in water or hydrocarbon solvents, respectively. Although many such silatrane derivatives are described in the literature, none have yet been investigated as coupling agents. Furthermore, as an additional novel aspect, mechanochemical, solvent-free reactions will be explored to align with green chemistry principles. Finally, applying these surface-treated fillers in 3D printing resin formulations will enable the study of how silatrane structure and deposition methods affect the properties of the resulting light-cured composites.

Expected results of the project

A wider aim of this project is to establish practical guidelines for facile surface functionalization with silatrane coupling agents, followed by comprehensive characterization—an approach that will be valuable for other research groups seeking well-defined organic–inorganic interfaces. Another anticipated benefit is the expansion of knowledge in silicon chemistry, driven by the synthesis and characterization of novel silatrane compounds. In addition, this research will contribute to advances in nanomaterial science by employing state-of-the-art analytical instruments to examine surface-treated nanofillers. Finally, the development of new resin formulations for 3D printing may reveal exceptional properties worthy of further investigation.