Nanohybrid LDH/GCN structures with conductive polymers: an innovative solution for photocatalytic water purification from estrogens in a flow-through reactor

Water pollution stems from many sources and causes negative changes in the physical, chemical, and biological properties of water. This often results from the introduction of excessive amounts of organic and inorganic compounds, radioactive materials, or even heat. Human activity plays the biggest role in this issue. As industry and agriculture expand and the global population grows, water quality continues to decline. Although wastewater from these activities undergoes treatment, current methods used in treatment plants are not always effective in removing all types of contaminants. **Estrogens** are example of such pollutants. They are natural and synthetic hormones that play a crucial role in the human body—but once they enter the environment, they become a growing concern. Even in tiny amounts (a few ng/L), estrogens can disrupt the hormonal balance of aquatic organisms, contribute to fish feminization and low sperm count in adult males. For humans, long-term exposure may lead to breast cancer, ovarian cancer, endometriosis, obesity, fibroids, and cardiovascular disease. This project focuses on two especially potent estrogens found in water: **estrone**, a naturally occurring compound, and **ethinylestradiol**, a synthetic hormone commonly used in contraceptive pills. These substances are highly active and stable, making them particularly difficult to remove from wastewater.

To tackle this problem, the project will use a process called **photocatalysis -** a method where materials absorb light and use that energy to break down pollutants. This method is regarded as environmentally friendly, as it breaks down pollutants during the reaction. It can be powered by various light sources - including sunlight, UV lamps, or visible light lamps, such as the commonly available LED bulbs proposed for use in this project. Photocatalysis is especially promising for removing estrogens because it doesn't just filter them out, it has the potential to destroy them at the molecular level. Effective photocatalysts must be able to absorb light and efficiently separate electrical charges (electrons and holes) to initiate chemical reactions. In this project, layered crystalline materials will be used, specifically **layered double hydroxides** (LDH) and **graphitic carbon nitride** (GCN). Both of these materials are known for their good charge transport properties and high surface area, making them suitable for capturing and breaking down pollutants that are hard to remove, like estrogens. These phases were combined with each other and **silver nanoparticles**, to form a composite material that will quickly perform a photocatalytic reaction.

Since real-world wastewater treatment involves constant water flow, the photocatalytic tests in this project will be performed in a **dynamic reactor** - a system designed to mimic the reaction in realistic conditions. The photocatalytic materials will be embedded in **polymeric beads** made out of **sodium alginate** to allow water to flow around them while keeping the material contained and reusable. To boost the performance of these beads, **conductive polymers** such as polypyrrole and polysulfone will be incorporated. These materials help shuttle charges during the photocatalytic process, enhancing the breakdown of estrogens when exposed to light. However, the degradation of estrogens doesn't always lead directly to **harmless by-products** like carbon dioxide and water. Sometimes, toxic intermediate compounds can be formed. To understand these transformations better, the project will **use density functional theory (DFT) calculations**, which is a **computational method** to model how molecules react under photocatalytic conditions. Then, the by-products will be analyzed **experimentally,** to compare the results to the calculations. This will help identify the degradation pathways and assess how safe the final products are.

In summary, **this project aims to develop advanced light-activated materials, shaped into polymer beads, to remove harmful estrogens from flowing water systems**. By combining experimental techniques with computer modelling, it will not only test how well these materials work, but **also understand exactly how the estrogens break down** - ensuring the process is both efficient and safe for the environment.