Title: Two Faces of Boron Cations: Merging Lewis Acid and Base Properties for Synthetic and Catalytic Applications

Transition metals dominate catalysis due to their ability to access multiple oxidation states and utilize filled and empty orbitals that are close in energy. However, their high cost, limited availability, toxicity, and environmental impact pose serious challenges for the future of sustainable catalysis. Therefore, attention should be paid toward the development of metal-free catalysts based on earth-abundant main-group elements. This project directly addresses that challenge by designing B-P systems that retain high reactivity while avoiding the drawbacks of transition-metal-based catalysis. According to the "main-group metallomimetics" concept, non-metallic systems can be engineered to mimic the key electronic properties of transition metals. The B-P cations studied in this project are specifically designed to exhibit ambiphilic character, enabling them to act as both electron-pair donors and acceptors in substrate activation. Low-coordination number of B-centre enhances the Lewis acidity and creates a site that is both electronically and sterically accessible for substrate binding. The phosphorus atom, being electron-rich, functions as a Lewis base. Despite the presence of a direct B-P bond, these cations retain distinct ambiphilic behaviour, making them unique among known cationic boron species. We anticipate that this combination of boron's intrinsic electron deficiency, coordinative unsaturation, and the proximity of a Lewis basic centre will promote the activation of strong chemical bonds under mild conditions. Moreover, the structural design of these systems may enable the activation of multiple small molecules simultaneously, opening new pathways for multi-site reactivity and metal-free catalysis. We aim to develop a library of B-P cations bearing substituents with varied steric and electronic properties. Preliminary studies indicate that even small changes in substitution patterns can significantly alter activation pathways. The reactivity of B-P cations will be tested against a range of environmentally and industrially relevant small molecules such as H_2, CO_2, N_2O, O_2, olefins, and carbonyl compounds. Building on these results, we plan to explore the catalytic application of B-P cations in hydroelementation reactions. This project will not only contribute to the development of new molecular-scale tools for small molecule activation but also support the broader goal of replacing traditional transition-metal catalysts with sustainable, metal-free alternatives. The small molecules targeted in this project play central roles in global challenges such as climate change, energy production, and pollution. Their selective activation and conversion into value-added products using main-group-based systems may contribute to addressing some of the most pressing problems facing modern chemistry and society.