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Design of selective reagents and functional materials: A theoretical and experimental approach

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The work illustrates the integration of basic and applied chemistry in the development and application of selective materials for application in desulfurization and denitrogenation of fuel as well as in separation of precious metals. The fuel chemistry study is important from the point of view of the need to drive towards a zero sulfur fuel as mandated by environmental protection agencies in many countries around the world.1 Challenges exist with the current hydrodesulfurization and hydrodenitrogenation processes that are being applied in refineries as they fail to achieve the requisite fuel standards. The second application of functional materials is in separation of important metals. The demand for precious metals is driven by their important applications, and the development of better separating reagents/materials has become important given that the quality of ores is decreasing, and better recovery rates of the metals from secondary sources (such as electronic boards and catalytic converters) will be required in future. This necessitates improvement of the current chemistry in order to process the new feeds.

Experimental and theoretical studies were carried out during the development of the functional chemistry for recognition of target metals and organic compounds. The selective chemistry towards fuel contaminants such as organosulfur and organonitrogen compounds has been developed, and the results are promising as the best material (polymenzimidazole nanofibers) achieve sulfur removal of less than 2 ppm.2 A process involving conversion of sulfur compounds to organosulfones compounds3 has been developed followed by removal of the polar sulfones using selective materials.2 The approach for materials development for metal ions, such as platinum group metals (PGMs), follows the development of reagents that are specific for metal ion chlorido complexes of interest. The innovation of the aforesaid reagents undoubtedly requires a design strategy that considers both the electronic and stereochemical requirements of the target anion. Through a combination of molecular modelling techniques and experimental techniques, we have been able to derive factors that lead to successful separations. Cations as anion receptors specific for [IrCl6]2- and [PtCl6]2^{-} will be presented as well as selective chemistry for orgnosulfur and organonitrogen compounds in fuel. Binding energies and other thermodynamic parameters have been calculated in silico to explain the chemistry involved.

References:

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