Expanding and Harnessing the Tunable Redox Nature of Dodecaborate Clusters

This work describes novel approaches to rationally tune the redox properties of icosahedral dodecaborate clusters through functionalization of all 12 boron vertices. Perfuctionalization in this manner engenders redox activity of the boron cluster derivatives, with the ability to tune these redox properties as a function of the substituent(s) used. New methods were developed to rapidly produce perfunctionalized boron clusters under ambient conditions, enabling accelerated development of additional cluster derivatives. Several clusters featuring higher redox potentials than any ether cluster derivatives to date were reported, extending the tunable range of B12(OR)12 clusters to over 1 V. Further modification of the cluster through vertex-differentiation by incorporating an NO2 group created a new class of B12(OR)11NO2 clusters with ~ 0.5 V higher redox potentials. After thorough demonstration of the high degree of redox tunability possible with these dodecaborate clusters, their extremely stable nature was shown via flow cell battery testing. The derivatives were tested in a symmetric cell, and a proof-of-concept all-boron flow cell battery prototype device was also demonstrated. In summary, several new methods to perfuctionalize dodecaborate clusters are reported, along with new insights on the significantly expanded available redox potential window for these clusters.

Boron-rich Clusters as Molecular Cross-linkers for Hierarchical Hybrid Materials

Cross-linking is important for materials to form rigid networks with improved thermal/mechanical properties. However, there exist a limited number of cross-linkers that are capable of generating rigid 3-dimensional networks and leading to significant changes of properties. Our group has recently developed a “molecular cross-linking” approach whereby a hybrid material is formed by cross-linking polyhedral boron cluster precursors, [B12(OH)12]2-, to the network of metal oxides using a simple solution-based synthesis. This new approach is enabled by the inherent robustness of the boron-cluster molecular building block, which is compatible with harsh conditions required for the synthesis of metal oxides. The unique structure of the hybrid material renders significantly enhanced electro- and photochemical property, evidenced by fast electron-transfer rates, low resistivity and photocatalysis under visible light conditions. Furthermore, we explored the possibility of cross-linking boron-rich clusters with organic molecules, such as diisocyanates and diboronic acids to form densely cross-linked polymeric materials. During the second portion of the seminar, I will describe these new polymeric materials as new architectures for diverse applications.

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