National Institute of Technology Rourkela

Registration Seminar

Seminar Title : In-Silico Investigations on the Structure, Dynamics and Solvation Properties of Efficient Magnesium Electrolytes
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Venue : Chemistry Department Seminar Room
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Abstract :

Magnesium-ion batteries offer several advantages over other metal-ion systems. Magnesium is earth-abundant, low-cost, and environmentally benign, addressing resource and sustainability concerns associated with lithium and cobalt-based chemistries. Its bivalent nature enables the transfer of two electrons per ion, potentially delivering higher volumetric energy density**.** Furthermore, Mg^{2+} exhibits a relatively high melting point and stability, making it suitable for long-cycle, high-temperature applications. These attributes position magnesium-ion batteries as a promising next-generation energy storage technology. While extensive research has focused on electrode and electrolyte materials, the electrolyte salt is equally critical in determining battery efficiency, stability, and ion transport. In this work, we designed and computationally evaluated magnesium salts incorporating &ndashCN and &ndashH functional groups to make organic heterocyclic-based superhalogen anions as a part of electrolyte salt for potential use in magnesium-ion batteries. Density Functional Theory (DFT) and classical Molecular Dynamics (MD) simulations have been employed to determine key electronic and structural parameters. The &ndashCN substitution markedly enhances electron affinity and binding strength, indicating improved redox stability compared to &ndashH analogues. Among the different heterocyclic halogen-based candidates, $Mg[C_4BN(CN)_5]_2$ demonstrated the most favorable superhalogen characteristics, with binding energies on par with commercial Mg salts. These results provide valuable guidelines for the rational design of next-generation magnesium electrolyte salts for multivalent battery technologies.