Title:	Functional hybrid solids for energy and medical applications
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Abstract:	Developing effective electrochemical conversion procedures is of great importance for storing and making use of renewable energy. Electrochemical oxygen evolution reaction (OER) plays a crucial role in many energy conversion technologies including CO2 reduction, metal–air batteries and complete water splitting. Unfortunately, the sluggish kinetics of OER required a high over-potential which hindered its efficiency. So, there exist a high requirement of effective electrocatalysts to facilitate OER effectively. Currently RuO2 and IrO2, are considered as the most effective electrocatalysts for OER. However, the large-scale application of these noble metal-based catalysts is limited by its high-cost and scarcity. The present thesis is focused on the development of functional hybrid materials and exploring their applications in water splitting and medicinal field. Metal–organic frameworks (MOFs) that are formed by organic ligands coordinated with metal atom nodes as periodic structural units possess tuneable nano porous structures and accessible, well-dispersed metal single sites, and present great potential for application as noble-metal-free water oxidation catalysts. We have synthesized two different architecture (2D and 3D) based cobalt-MOFs and explored their activity for OER. 2D MOF shows an extraordinary OER performance with 175 mV overpotential to achieve 10 mA cm-2 current density and low Tafel slope value of 80 mV/dec, whereas 3D MOF needed an overpotential of 389 mV to attain 10 mA cm-2 current density. Polyoxometalates (POMs) constitute a family of nanomaterials, which offer tremendous potential for a range of energy-related applications. Their certain properties like (1) POM clusters are conductive to exposing more catalytically active sites. (2) POM-based compounds usually demonstrate reversible multi-electron redox transformations while keeping stable structures. (3) POM molecules can be bridged with organic ligand or confined into pores to form POM-based inorganic-organic hybrid materials with atomically accurate and equally distributed active sites, make them suitable for water splitting applications. We have synthesized an Anderson cluster based functional hybrid solid which shows efficient activity towards OER, also, its performance and stability was enhanced by making its composite with Acetylene black. This attempt provides a new vision for enhancing the OER performance of POM based materials. POMs, which are designated as clusters of transition metal (W, Mo, V, Nb) and oxygen atoms, have been discovered to be promising anticancer drug candidates in recent decades. According to the World Health Organization, cancer is one of the leading causes of death worldwide, accounting for 8.8 million deaths in 2015. Cisplatin (CDDP), the most well-known cytotoxic drug class, is still one of the frequently used chemotherapeutic agents in clinics. Aside from CDDP, a number of other drugs have demonstrated anticancer potential by temporarily alleviating symptoms, extending patients' lives, and, in rare cases, curing cancer. All of them, however, have certain limitations and severe side effects due to a lack of selectivity, low efficacy against certain cancer types, and low bioavailability. As a result, the search for another drugs that selectively incapacitate cancer cells while causing minimal harm to normal cells continues. POMs' anticancer activity was first revealed in 1965, when Mukherjee defined the in vivo application of PTMC, a mixture of H3[PW12O40], H3[PMo12O40], and caffeine, on patients suffering from gastrointestinal cancer. Despite the fact that it results in the complete disappearance of tumors, PTMC was not continued to further clinical trials. Years later, in 1974, Jasmin et al. reported that (NH4)17Na[NaSb9W21O86] inhibited sarcoma virus-induced tumours. Since then, much importance has been placed on the advancement of biologically active POMs. We have synthesized two new polyoxomolybdate cluster based hybrid solid namely an Octamolybdate cluster based solid, [(Cu(pic)2)2(Mo8O26)]·8H2O and a Strandberg type polyoxomolybdate based hybrid solid, [{4,4'-H2bpy}{4,4'-Hbpy}2{H2P2Mo5O23}]·5H2O. The In vitro anti-tumoral activity of both the solids has been tested against human breast cancer (MCF-7), lung cancer (A549) and liver cancer (HepG2) cells. Octamolybdate-based solid yielded the lowest IC50 value reported so far among octamolybdate anion-based hybrid solids, i.e., 24.24 μM for MCF-7, 21.56 μM for HepG2, and 25 μM for A549, indicating significant anti-cancer activity. The cell cycle analysis further reveals the observed anti-tumor effect to be governed by the arrest of breast cancer cells in the G2/M phase while that of lung and liver cancer cells in the S phase of the cell cycle. A fluorescence quenching study suggests the binding interaction between solid and ctDNA, which in turn induces apoptosis and necrosis pathways leading to cancer cell death. The Strandberg type cluster was used against the MCF-7 and A549 cancer cells for the first time. It shows considerable inhibitory effect with IC50 values of 33.79 μM, 25.17 μM, and 32.11 μM against HepG2, A549 and MCF-7 respectively. The anti-tumoral activity was also found to be comparable with that of a well-established chemotherapeutic agent, methotrexate (MTX). A novel molybdenum-based coordination polymer, [Mo2(μ2-O)O4(2-pyc)2(H2O)], was also synthesized. This Mo coordination polymer was found to show a considerable inhibitory effect with IC50 values of 22.63 μM, 28.19 μM, and 20.97 μM, against HepG2, A549, and MCF-7 cell lines respectively. This was the first attempt at exploring the molybdenum-based coordination polymer for antitumor applications.
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