

P1.40 Core-shell Zn-Co zeolitic imidazolate frameworks as efficient catalysts for the reverse water-gas shift reaction

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Abstract

The reverse water-gas shift (RWGS) reaction has attracted growing interest as an effective route for converting carbon dioxide (CO₂) into carbon monoxide (CO), a valuable precursor for downstream chemical synthesis. In this study, Zn-Co zeolitic imidazolate frameworks (ZIFs) with core-shell architectures were synthesized and evaluated as catalysts for the RWGS reaction. Core-shell structures, namely ZIF-67@8 and ZIF-8@67, were successfully prepared and compared with bare ZIF-8 and ZIF-67. Structural and physicochemical properties were investigated using X-ray diffraction, thermogravimetric analysis, SEM-EDX, TEM, and X-ray absorption spectroscopy (XAS), including time-resolved XAS during thermal pretreatment. Characterization results confirmed the formation of well-defined core-shell morphologies with preserved ZIF crystallinity prior to thermal treatment. Time-resolved XAS revealed that cobalt species in all samples transformed into the metallic phase at approximately 600 °C, while zinc remained as Zn²⁺ (ZnO). Catalytic evaluation demonstrated that pretreatment temperature strongly influenced activity and selectivity. Core-shell catalysts pretreated at 700 °C exhibited enhanced CO₂ conversion (up to ~60%) and higher CO yields compared to bare and non-core-shell samples, with CO as the dominant product. The superior performance is attributed to improved dispersion of active cobalt sites and defect sites generated from ligand decomposition. These findings demonstrate the potential of core-shell Zn-Co ZIFs as efficient catalysts for CO₂ conversion via the RWGS reaction.

Keywords

Reverse water-gas shift
Core-shell zeolitic imidazolate frameworks
CO₂ conversion

P1.41 Materials-microorganism interfaces: toward engineered living coating systems

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Abstract

Materials-microorganism interfaces play a central role in the development of engineered living coating systems for sustainable architectural applications. However, interactions between microorganisms and solid construction materials, particularly involving fungal systems, remain poorly understood.

Aureobasidium pullulans, a yeast-like, non-pathogenic environmental fungus capable of colonising a wide range of surfaces, was selected as a model organism for its relevance to living coating applications. In this study, various surfaces, including wood and mineral substrates, as well as model gold nanoparticles (AuNPs), were investigated to reveal their interactions with fungal cells. Wood-based and concrete materials were selected as representative construction substrates, while AuNPs were introduced as a model nanoscale system to enable comparison between nanoparticle interactions with bacterial and fungal cells. This approach serves as an initial step toward extending DLVO theory, previously applied to bacteria-nanoparticle systems, to more complex microorganism-material interfaces.

A multiscale microscopic approach was applied to examine microbial attachment, interface formation, biofilm organization, and interactions between nanoparticles and microbial cells. The results reveal substrate-dependent differences in colonization, including variations in hyphal network development, surface coverage, and nanoparticle attachment to cell surfaces.

These findings provide new insight into materials-microorganism interactions across multiple length scales and highlight the role of surface properties in governing colonization and interface formation. This work establishes a framework for studying such interfaces and supports the design of bioinspired and engineered living coatings.

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Keywords

living coating
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P1.42 Effects of pulverization on corrosion kinetics and interfacial reactions of CLF-1 steel with Li₄SiO₄ tritium breeder pebble

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Abstract

The corrosion kinetics and interfacial reactions of CLF-1 steel with LiSiO tritium breeder pebbles was systematically investigated at high-temperature breeding blanket conditions. The results demonstrate that the corrosion process progressively evolves from localized corrosion dominated by pebble-steel contact regions at the early stage to nearly uniform corrosion with increasing exposure time. This transition is closely associated with the formation, cracking, and pulverization of LiSiO / LiCO surface layers on LiSiO pebbles, which significantly enhance interfacial corrosion. A multilayer corrosion structure consisting of a Fe-rich outer layer, an intermediate Fe-Cr mixed layer, and a dense Cr-rich inner layer was formed on the steel surface. Thermodynamic modeling confirmed that the interfacial reaction mechanism involves oxidation and lithiation reactions. TEM observations revealed the dynamic microstructural evolution and phase transformations responsible for the formations of the multilayer corrosion architecture. The corrosion kinetics follow a parabolic rate law, indicating that the long-term corrosion is controlled by diffusion through the Cr-rich inner layer.

Keywords

CLF-1 steel
Li₄SiO₄
interfacial corrosion
fusion blanket

P1.43 Multiscale evaluation of thermo-mechanical response and microstructural stability of Hastelloy nickel-based alloys at elevated temperatures

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Abstract

Nickel-based Hastelloy alloys are widely applied in high-temperature structural components due to their excellent thermal stability, corrosion resistance, and mechanical performance. In this study, a comprehensive evaluation of the thermo-mechanical and surface-related behaviour of selected commercial alloys—Haynes 230, Hastelloy B-3, Hastelloy C-276, Hastelloy N, and Hastelloy X—was conducted over a temperature range from room temperature up to 1050°C. Particular attention was devoted to temperature-induced microstructural evolution and surface-related degradation mechanisms affecting thermo-mechanical performance. The temperature-dependent coefficient of thermal expansion was determined using dilatometry, while thermal diffusivity and specific heat capacity were measured by the Laser Flash method and simultaneous thermal analysis (STA), respectively. Local and bulk mechanical responses were assessed through high-temperature nanoindentation and tensile testing performed as a function of temperature, enabling direct correlation between surface-scale and macroscopic mechanical behaviour. Microstructural evolution and surface-related degradation mechanisms induced by high-temperature exposure were investigated using scanning electron microscopy (SEM) before and after thermal loading. The results reveal distinct temperature-dependent changes in thermal transport properties, mechanical response, and microstructural stability among the investigated alloys, highlighting the role of surface and subsurface phenomena in high-temperature performance. The combined experimental approach provides valuable insight into the reliability of Hastelloy alloys under extreme thermal conditions and supports their selection for advanced high-temperature and nuclear energy applications.

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