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ABSTRACT:

Monte Carlo Simulation in Nanomaterial Research: Advancements, Applications, and Future Prospects in Nanocatalysis and Nanostructures

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Monte Carlo Simulation (MCS) is a fundamental computational tool in nanomaterials research, providing deep insights into the behaviour and properties of materials at the nanoscale. This review discusses recent advances and applications of MCS, emphasizing its crucial role in nanocatalysis and the investigation of fundamental catalytic material properties [1-2]. In particular, MCS enables detailed exploration of the nature and characteristics of active sites, offering a powerful approach to unravelling atomic-scale interactions, adsorption dynamics, and reaction pathways in heterogeneous catalysis. By providing a robust framework to model complex phenomena that traditional methods often struggle to capture, MCS has become nowadays indispensable across multiple research fields. One key application of MCS is in modelling kinetic processes, and catalytic reactions at the nanoscale, shedding light on adsorption-desorption mechanisms, reactant diffusion on catalyst surfaces, and reaction energetics [2]. Such studies are fundamental in identifying highly active and selective catalytic sites, ultimately guiding the design of next-generation catalysts with enhanced performance and stability. MCS also excels in simulating complex atomic interactions and predicting material behaviour, which is crucial for designing nanomaterials with tailored, high-performance characteristics. In the field of nanocatalysis, MCS has proven to be particularly powerful in revealing atomic-scale structural patterns, nanoparticle sintering dynamics, and interactions with catalytic support, all of which, ultimately, govern catalytic activity and selectivity [3].

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