Chapter 7
Advanced Studies on Hydrogen Energy Using Computational Chemistry

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ABSTRACT

The paper examines the latest optimization models for the hydrogen transportation and production. Optimization plays a crucial role in systematic methodologies that aid in hydrogen expansion. Energy for most systems comes from non-renewable sources like fossil fuels, which take a long time to recharge and never quite reach their full potential. Energy problems, climate change, and environmental degradation have all resulted from the widespread usage of fossil fuels. One of the many benefits of hydrogen is its abundance of clean, efficient sources. In order to back up hydrogen expansion, systematic techniques must include optimization. Some of the recent developments in the transportation, storage, and generation of hydrogen are covered, including the use of clean processes such as photo electrolysis, water electrolysis, pyrolysis, and partial oxidation. Researchers interested in applying optimization approaches to hydrogen supply chain networks may find this study to be a useful blueprint.

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1. INTRODUCTION

Hydrogen has been a popular subject in discussions about fueling the transportation industry since the 1970s. However, its use has been limited due to the significant investment and production costs, as well as the presence of more affordable fuel options(Bockris, 2013). With the increasing demand for countries to lower the release of greenhouse gases and transition to cleaner fuels, hydrogen has resurfaced as a possible energy carrier. This can serve as an alternative to petroleum-based fuel in industries like stainless steel, heat and chemicals, where lowering transmission has traditionally posed challenges(Kwok, 2021). Within the chemical sector, there have been proposals to utilize "electrolyzer" and CCS (carbon capture and storage) technologies to decrease emissions associated with ammonia production by substituting hydrogen with cleaner options (*Global Hydrogen Review 2022*, 2022). Hydrogen plays a crucial role in improving the reliability, sustainability, and adaptability in energy systems, while also supporting the addition of clean energy sources in the power sector. This can be manufactured in areas with abundant non-exhaustible resources and then delivered over long distances to nations with high energy needs as well as scarce materials. As of the year 2021, a total of seventeen nations, including Germany, Japan(Meti & Dabburu, 2017), and 'South Korea', were already developing hydrogen strategies for the gradually rollout of new usage, infrastructures technical as well as institutional production of hydrogen, and trade rules. At present, most of the hydrogen production comes from fossil fuels using steam methane reformation (SMR) (Irena., 2019).The primary challenges in advancing a hydrogen economy are the absence of green hydrogen production facilities and the inadequate hydrogen storage and transportation infrastructures. Developing investment strategies is essential for advancing research in low-carbon hydrogen technologies and supporting their widespread adoption in different industries(*Global Hydrogen Review 2022*, 2022). The objective is to reduce the price of hydrogen with low emissions to competitive levels within ten years, as set by the USA's Department of Energy(SANBORNSCOTT, 2004). Hydrogen could potentially revolutionize the energy sector and the economy due to its important role in electrical systems, transportation, and manufacturing industries. The energy sector operates in a complex web of interdependence, as energy serves as the foundation of industrialized economies. Hydrogen's emergence as a new energy source could signifies the prices of economies and other energy sources. In the 1970s, there was a significant increase in global oil prices, resulting in stagflation, economic expansion, and elevated inflation levels("International Energy Agency (IEA)," 2008). When considering the significance of extending a hydrogen supply chain on the economies of countries involved in hydrogen production and consumption, two key areas of research are the development of the the hydrogen supply chain