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Molecular dynamics simulations in membrane-based water treatment processes: A systematic overview

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ABSTRACT

A thorough investigation of membranes as well as their transport and material properties is a key to understanding the governing principles and unresolved issues of membrane processes. Through molecular dynamics (MD) simulations, static and dynamic properties of membrane separation systems may be investigated on a molecular level. By reviewing over 70 articles, this paper aims to highlight the usefulness of applying molecular dynamics in membranes (MDM) in order to broaden our knowledge of membrane-based water treatment processes. Here, the theoretical foundations of classical MD are described together with the results that are obtainable from MDM simulations. By compiling results from published works, we emphasize the ability of MD to determine membrane transport and material properties from simulations. The authors conclude by suggesting the further use of MDM for prospective research areas pertaining to membrane-based water treatment processes.

Contents

1. Introduction

Due to the growing concerns about the availability of water, researchers are currently searching for more efficient ways of obtaining clean and safe drinking water and maintaining the quality of freshwater sources, without causing further environment and energy issues. As a solution to these challenges, membrane-based water treatment processes have become relevant in recent decades because of their ability to improve water

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