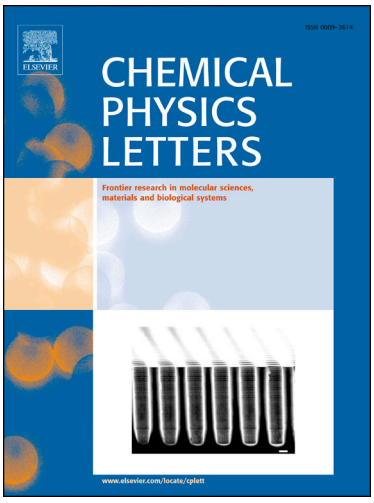

Research paper

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A new method for finding the minimum free energy pathway of ions and small molecule transportation through protein based on 3D-RISM theory and the string method

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ABSTRACT

A new method for finding the minimum free energy pathway (MFEP) of ions and small molecule transportation through a protein based on the three-dimensional reference interaction site model (3D-RISM) theory combined with the string method has been proposed. The 3D-RISM theory produces the distribution function, or the potential of mean force (PMF), for transporting substances around the given protein structures. By applying the string method to the PMF surface, one can readily determine the MFEP on the PMF surface. The method has been applied to consider the Na^+ conduction pathway of channelrhodopsin as an example.

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