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作成：弘前大学附属図書館資料管理G雑誌情報担当

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Expansive Quantum Mechanical Exploration of Chemical Reaction Paths

Alberto Baiardi, Stephanie A. Grimmel, Miguel Steiner, Paul L. Türtischer, Jan P. Unsleber, Thomas Weymuth, and Markus Reiher*

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SUBJECTS: Molecular dynamics, Chemical structure, Algorithms, Chemical reactions, ∨

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Abstract

Conspectus

Quantum mechanical methods have been used for the elucidation of reaction paths of chemical reactions.

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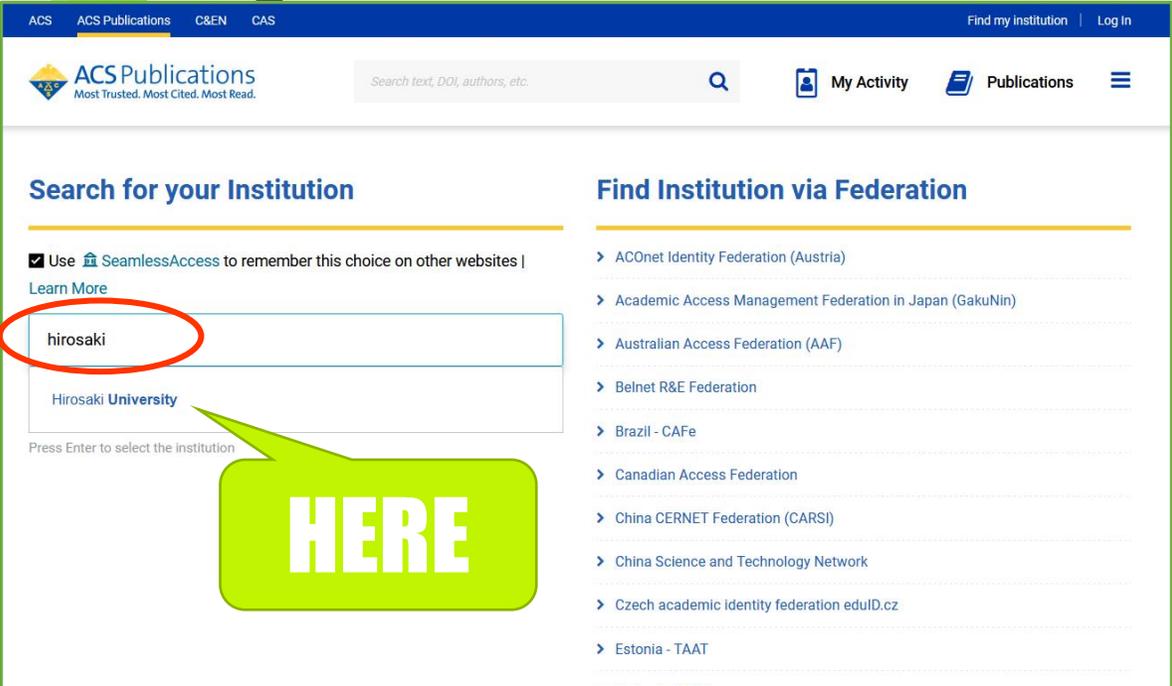
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