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Fragment-Based Quantum Mechanical/Molecular Mechanical Simulations of Thermodynamic and Kinetic Process of the Ru²⁺-Ru³⁺ Self-Exchange Electron Transfer

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JOURNAL OF CHEMICAL THEORY AND COMPUTATION

Volume: 8 Issue: 12 Pages: 4960-4967

DOI: 10.1021/ct300758v

Published: DEC 2012

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Abstract

A fragment-based fractional number of electrons (FNE) approach is developed to study entire electron transfer (ET) processes from the electron donor region to the acceptor region in the condensed phase. Both regions are described by the density-fragment interaction (DFI) method, while FNE as an efficient ET order parameter is applied to simulate the electron transfer process. In association with the QM/MM energy expression, the DFI-FNE method is demonstrated to describe ET processes robustly with the Ru²⁺-Ru³⁺ self-exchange ET as a proof-of-concept example. This method allows for systematic calculations of redox free energies, reorganization energies, electronic couplings and the absolute ET rate constants within the Marcus regime.

Keywords

KeyWords Plus: DENSITY-FUNCTIONAL THEORY; MOLECULAR-DYNAMICS SIMULATION; REORGANIZATION FREE-ENERGIES; 4-HELIX BUNDLE PROTEIN; TRANSFER RATES; TUNNELING PATHWAYS; REDOX REACTION; LARGE SYSTEMS; HOLE TRANSFER; AB-INITIO

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Funding

Funding Agency	Grant Number
National Institute of Health	NIH R01-GM061870 P50GM067082
U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences	DE-SC0001011
HPC Advisory Council	

[View funding text](#)

Publisher

AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

Categories / Classification

Research Areas: Chemistry; Physics

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Document Information

Document Type: Article

Language: English

Accession Number: WOS:000312122200013

PubMed ID: 23682243

ISSN: 1549-9618

eISSN: 1549-9626

Journal Information

Table of Contents: [Current Contents Connect](#)

Impact Factor: [Journal Citation Reports](#)

Other Information

IDS Number: 051JJ

Cited References in Web of Science Core Collection: **77**

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