Accepted Manuscript

Constant-potential molecular dynamics simulations on an electrode-electrolyte system: calculation of static quantities and comparison of two polarizable metal electrode models

Yusuke Matsumi, Hiroshi Nakano, Hirofumi Sato

Please cite this article as: Y. Matsumi, H. Nakano, H. Sato, Constant-potential molecular dynamics simulations on an electrode-electrolyte system: calculation of static quantities and comparison of two polarizable metal electrode models, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.05.032

Constant-potential molecular dynamics simulations on an electrode-electrolyte system: calculation of static quantities and comparison of two polarizable metal electrode models

Yusuke Matsumi[a], Hiroshi Nakano[a,b,*], Hirofumi Sato[a,b]

[a]*Department of Molecular Engineering, Kyoto University, Kyoto 615-8510, Japan.*
[b]*Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Nishikyo-ku Kyoto 615-8510, Japan.*

Abstract

We investigated a Pt electrode-water molecules system by constant potential molecular dynamics simulations using two different models for electronically polarizable metal electrodes. Static quantities were calculated such as the number density profiles, electrostatic potential profiles, and the potential of mean force profiles for the approach of a Na^+ to an electrode. The two models were compared to find out they give results in good agreement with each other. The electrostatic potential acting on the Na^+ was also evaluated and decomposed to get insight into the importance of the interactions between a redox species and polarizable metal electrodes.

Keywords: electrode-electrolyte system, constant potential molecular dynamics, polarizable electrode

1. Introduction

Theoretical study on a redox process in an electrochemical cell is very challenging. One of the reason is the difficulty in describing the complex interactions present in the electrode-electrolyte system. In addition to the large solvation

---

[*]Corresponding author
URL: hnaka@moleng.kyoto-u.ac.jp (Hiroshi Nakano)