

Author's Accepted Manuscript

Theoretical prediction of the local structures and transport properties of binary alkali chloride salts for concentrating solar power

Jing Ding, Gechuanqi Pan, Lichan Du, Jianfeng Lu, Xiaolan Wei, Jiang Li, Weilong Wang, Jinyue Yan



PII: S2211-2855(17)30433-0
DOI: <http://dx.doi.org/10.1016/j.nanoen.2017.07.020>
Reference: NANOEN2078

To appear in: *Nano Energy*

Received date: 7 June 2017
Accepted date: 10 July 2017

Cite this article as: Jing Ding, Gechuanqi Pan, Lichan Du, Jianfeng Lu, Xiaolan Wei, Jiang Li, Weilong Wang and Jinyue Yan, Theoretical prediction of the local structures and transport properties of binary alkali chloride salts for concentrating solar power, *Nano Energy*, <http://dx.doi.org/10.1016/j.nanoen.2017.07.020>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain

Theoretical prediction of the local structures and transport properties
of binary alkali chloride salts for concentrating solar power

Jing Ding¹, Gechuanqi Pan¹, Lichan Du¹, Jianfeng Lu¹, Xiaolan Wei², Jiang Li³, Weilong Wang^{1*}, Jinyue Yan^{4,5}

¹*School of Engineering, Sun Yat-Sen University, Guangzhou 510006, PR China*

²*School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, PR China*

³*National Supercomputer Center in Guangzhou, Guangzhou 510006, PR China*

⁴*School of Business, Society and Energy, Mälardalen University, Västerås, Sweden*

⁵*Energy Process Division, Royal Institute of Technology, Stockholm, Sweden*

*Corresponding author. wwlong@mail.sysu.edu.cn(WL Wang)

Abstract

Comprehensive molecular simulations have been carried out to compute local structures and transport properties of different components of binary NaCl-KCl over a wide operating temperature range. The partial radial distribution functions, coordination number curves and angular distribution functions were calculated to analyze the influence of temperature and component on local structures of molten Alkali Chlorides. Transport properties were calculated by using reverse non-equilibrium molecular dynamics (RNEMD) simulations including densities, shear viscosity and thermal conductivity. The results show that ion clusters are considered to be formed and the distance of ion clusters become larger with increasing temperature which has great

Download English Version:

<https://daneshyari.com/en/article/5452375>

Download Persian Version:

<https://daneshyari.com/article/5452375>

[Daneshyari.com](https://daneshyari.com)