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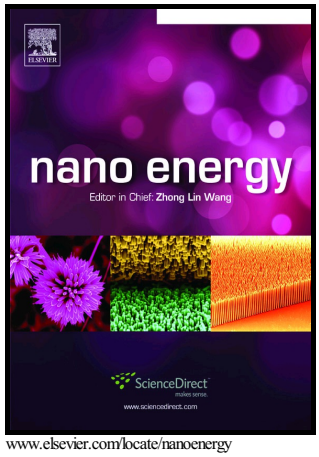

www.elsevier.com/locate/nanoenergy

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, Xiaola Wei, Jiang Li, Weilong Wang and Jinyue Yan, Theoretical prediction of the local structures and transport properties of binary alkali chloride salts for concentratin solar power, *Nano Energy,* http://dx.doi.org/10.1016/j.nanoen.2017.07.020

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

Jing Ding[1], Gechuanqi Pan[1], Lichan Du[1], Jianfeng Lu[1], Xiaolan Wei[2], Jiang Li[3], 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