Amir Zareian Jahromi, J Material Sci Eng 2014, 3:3
http://dx.doi.org/10.4172/2169-0022.S1.016

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference and Exhibition on
Materials Science & Engineering
October 06-08, 2014 Hilton San Antonio Airport, USA

A transport model for thermodynamic estimation of cryogenic hydrogen

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Hydrogen is a foundation element of the universe and has attracted attention as a key of the solution for the energy and environmental problem. However, liquid hydrogen shows strange behavior as compared to other field due to the nuclear quantum effect. Because of this effect it is difficult to comprehend the thermodynamic and transport properties of liquid hydrogen by using the usual method. Therefore several methods have been proposed to reproduce the time evolution of the molecules in which the nuclear quantum effect contributes to their behavior. However, since the previous studies are still verification stage of the methods, an effect of the nuclear quantum nature of hydrogen and its mechanism on the thermodynamics and transport properties have not been clarified in details. Especially, how the quantum nature would effect on the energy transfer in molecular scale has not been clarified. In this study, therefore, we investigated the effect of this quantum nature and its mechanism on the thermodynamics and transport properties of cryogenic hydrogen using classical molecular dynamics (MD) methods. We applied Centroid Molecular Dynamics (CMD) methods, Ring Polymer Molecular Dynamics (RPMD) methods, and Maximum Entropy numerical analytic continuation (MEAC) methods. First, we have conducted thermodynamics estimation of cryogenic hydrogen using the MD methods. As a result, it was confirmed, that both quantitative and qualitative effect of the quantu.

Biography

Amir Zareian Jahromi has completed his MSc at the age of 27 years from university of Tehran and starts his new program in management and business administration. He is the executive manager of Danesh Pajoohan Company in Iran, and is in cooperation with international companies in electrical engineering and bioelectronics.

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