



Contribution ID: 19

Type: Poster Presentation

Investigation of the radiation emission influence on properties of liquid water systems

Monday, 11 July 2016 16:30 (1 hour)

Abstract content
 (Max 300 words)
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Present work is dedicated to the investigation of the radiation emission influence on those thermodynamic properties of liquid water systems, which are defined by the change of chemical potential of the liquid and its components under the influence of radiation. It was shown, that irradiation of the coexisting phases in stationary state results in the shift of the phase transition points parameters. The shift of temperature and pressure of phase transitions of the first order under the influence of radiation was evaluated taking in count both entropy and interaction factors at the chemical potential of the regarded system. Also we present the first step of a general study on induced radiation damage by 256 water molecules in simulation box at $T=(280-315)$ K at the molecular level by MD. The main goal of this work is to study the water structure, thermodynamics and dynamics changing under induced by the radiation damage from 0.1 keV to 1MeV.

The MD codes used in this study includes all

relevant interactions (cluster formation) and dynamics properties (MSD, VAF and diffusion) to obtain structure and dynamics properties systems of study under radiation damage.

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Session Classification: Poster Session