18th Annual City Tech Poster Session

QUASI-PHASE STATES OF MOLECULAR SYSTEMS

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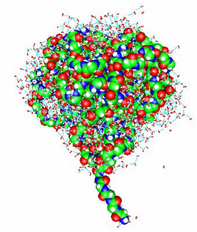

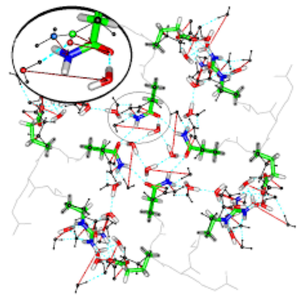

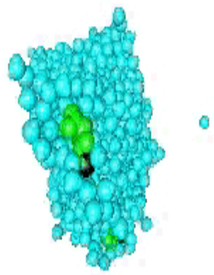

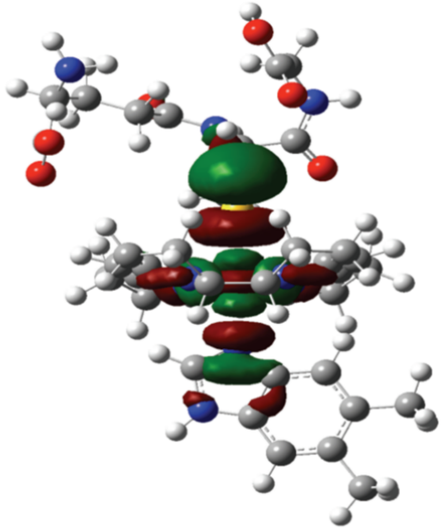

Molecular Dynamics and Quantum Chemistry studies for ionic systems [1,2], water [3], and biological macromolecules [4] revealed numerous quasi-equilibrium **quasi-phase** states. For example, macroscopic phase transitions are chaotic numerous jumps of nanoscale clusters between numerous quasi-phase states.

The concept of quasi-phase states, which depend on the system configuration and boundary conditions, is useful to describe nanoscale and surface phenomena. At temperatures of the bulk liquid phase, these quasi-phase states can have solid's properties, and vice versa, as in the contact-melting phenomenon. Nanoscale biological phenomena, as mechanisms of ion channels, can be explained in terms of quasi-phases. Further research should be aimed at identifying specific quasi-phase states of various systems. For example, the penetration of virus molecules through cell membranes can be studied as membrane quasi-melting in the place of penetration.

1. Molecular Dynamics Study of Ionic Melts Resulting from Contact Melting.
E. A. Goncharenko,… Inorganic Materials, Vol. 36, No. 10, 2000, pp. 1056–1059.
2. Molecular Dynamics Study of Polarity in Room-Temperature Ionic Liquids
Vasiliy Znamenskiy and Mark N. Kobrak. The Journal of Physical Chemistry B 2004 108 (3), 1072-1079
DOI: 10.1021/jp035891m
3. Quantum Calculations On Hydrogen Bonds In Certain Water Clusters Show Cooperative Effects. Znamenskiy VS, Green ME. J Chem Theory Comput. 2007 Jan;3(1):103-114.
4. Quantum mechanical calculations of charge effects on gating the KcsA channel. Alisher M Kariev 1, Vasiliy S Znamenskiy, Michael E Green, Biochim Biophys Acta. 2007 May;1768(5):1218-29.