

Nucleation and growth of methane clathrate hydrate crystal - molecular dynamics study

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Clathrate hydrates (CH) are solid structures formed by water molecules organised in cages. Inside those cages guest molecules are encapsulated. Vast amounts of methane CH's found in marine sediments and in permafrost regions may become important source of natural gas in near future. However, still little is known about the exact mechanism of their formation and dissociation what hinders development of extraction technologies.

To fill this gap several molecular dynamics simulations of the systems containing methane dissolved in liquid water were performed. Layers of the clay were attached to the rectangular unit cell to represent the natural environment in which hydrates are being formed. The role of the temperature, concentration of methane, ionic strength of the solution and type of clay on the nucleation process was considered. Microsecond range of trajectory was collected in nVT ensemble for systems containing about 16000 atoms using TIP4P2005 for water, single L-J site for methane and CLAYFF for clay atoms.

Picture below depicts system containing water solution of methane (with methane concentration equal to 25% of methane concentration found in hydrate) after 1245ns of trajectory. Nucleation center was formed close to pyrophyllite clay surface.

