



Contribution ID: 2 Contribution code: Board 55

Type: Poster Presentation

## Molecular mechanisms of water intrusion and extrusion in hydrophobic nanopores

*Monday, May 20, 2024 7:10 PM (20 minutes)*

**ABSTRACT:** Lyophobic nanoporous particle suspensions are being explored as promising materials for energy absorption and storage. In these systems, known as nanoscale energy absorption systems (NEAS), the non-wetting solvent intrudes into nanopores when subjected to mechanical compression, converting and storing the impact energy that can be further released upon solvent extrusion when the compression force is removed.<sup>1</sup> While various NEAS have been explored experimentally, the molecular level mechanisms of the intrusion-extrusion cycles are not well-understood. Using atomistic molecular dynamics simulations (MD), we investigate the dynamics of shock impact induced intrusion and extrusion of water in hydrophobic cylindrical channels. MD simulations performed for nanopores of different sizes at quasi-static and dynamic conditions demonstrate three different stages of the compression process: (1) initial elastic compression of the solvent, (2) fluid intrusion into the pore upon reaching a threshold intrusion pressure and (3) elastic compression of the solvent upon pore-filling (see Fig. 1). Extrusion of the solvent from a completely filled nanopore upon the release of pressure is initiated by the bubble nucleation. Our simulation results are correlated to the experimental observations. <sup>1</sup>

<sup>1</sup> Belogorlov, Anton A., et al. "Suspensions of lyophobic nanoporous particles as smart materials for energy absorption." *Journal of Colloid and Interface Science* 600 (2021): 229-242.

Indico rendering error

Could not include image: [403] Error fetching image

**Primary authors:** Mr ABDELLA, Abdelraheem (Rutgers, The State University of New Jersey); Dr SANTO, Kollattukudy P. (Rutgers, The State University of New Jersey); Mr NEIMARK, Alexander (Rutgers, The State University of New Jersey)

**Presenter:** Mr ABDELLA, Abdelraheem (Rutgers, The State University of New Jersey)

**Session Classification:** Poster Session

**Track Classification:** Poster Presentations