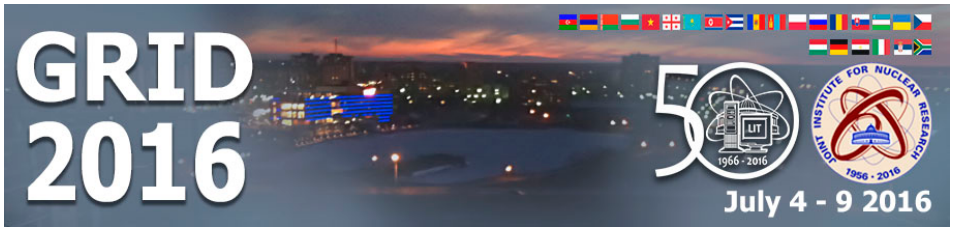

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HPC design of ion based molecular clusters

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Different self-assembled molecular clusters grown around H+ and Na+ ion kernels have been investigated using density functional theory method considering advanced exchange-correlation DFT functionals. Supramolecular structures of high-order molecular associations observed in different mass spectra and their formation dynamics were explained with the help of HPC technique. The presence of new and unusual weak intermolecular forces which keep together these supramolecular assemblies were observed and characterized in more details using molecular modeling methods.

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