Nanoscale physics

Computer simulation of collision-induced spectra of confined argon-xenon mixture

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Molecular dynamics method has been used to simulate the interaction induced absorption in argon-xenon binary mixtures confined between graphite walls. The graphite walls have been represented as the rigid bodies without internal degrees of freedom. The calculations have been made for the various percentage compositions of binary mixtures at the constant density and total number of atoms. The interaction induced dipole moment of a colliding pair was represented by phenomenological formula available in the literature [1]. Both the many-body correlation functions and the corresponding spectra were simulated for several temperatures (T=50-140 K). The substantial differences between the spectra of confined and bulk mixtures have been observed.

Figure 1. The instantaneous configuration of the argon-xenon mixture between graphite walls at T=110.0 K

1. *Dawid A., Gburski Z.* Interaction-induced absorption in argon-krypton mixture clusters: Molecular-dynamics study// Physical Review A.-1997.-**58.**-P. 740-743.