MOLECULAR DYNAMICS SIMULATIONS OF ASYMMETRIC COLLOIDAL BINARY MIXTURES

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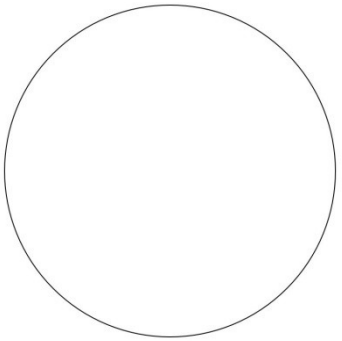
Introduction

- Wide variety of systems with asymmetry in mass, size, charge and their combinations were studied.
- Each system was studied from the point of view of their equilibrium structure and transport properties.
- Simulation time varied from 3.4 ns to 18 ns depending upon the system with a time step of 6 fs.
- Properties calculated:

1. Equilibrium Properties like Energy ,pressure etc
2. Radial Distribution Function
3. Structure Factor
4. Van Hove Autocorrelation Function

AIM

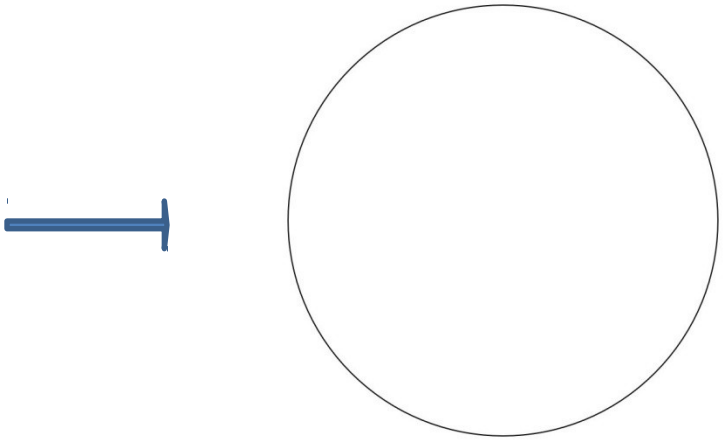
Symmetric Colloidal Mixture



Type 0

Type 1

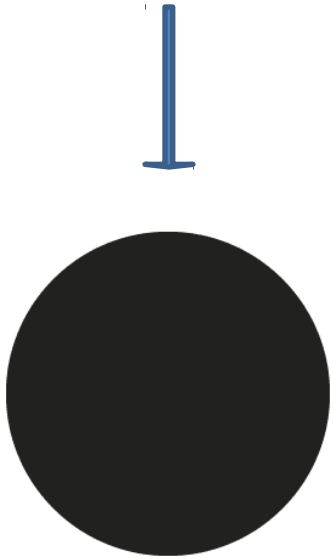
Size Asymmetry



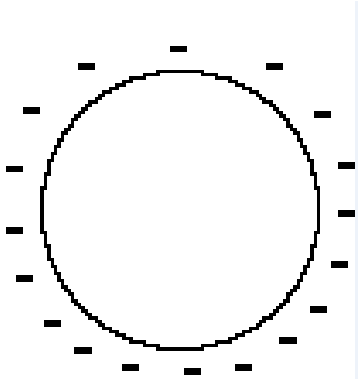
Type
0

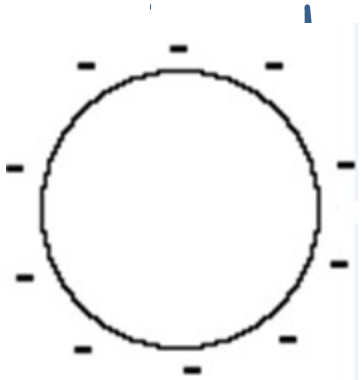
Mass Asymmetry

Type 0

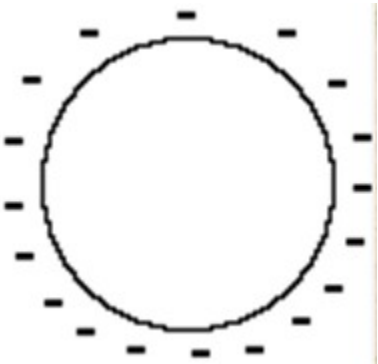


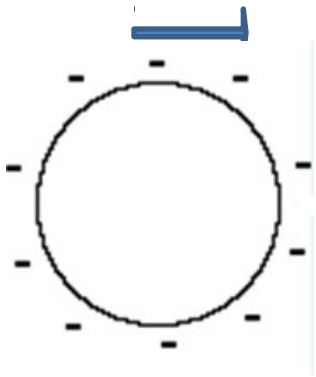
Charge Asymmetry

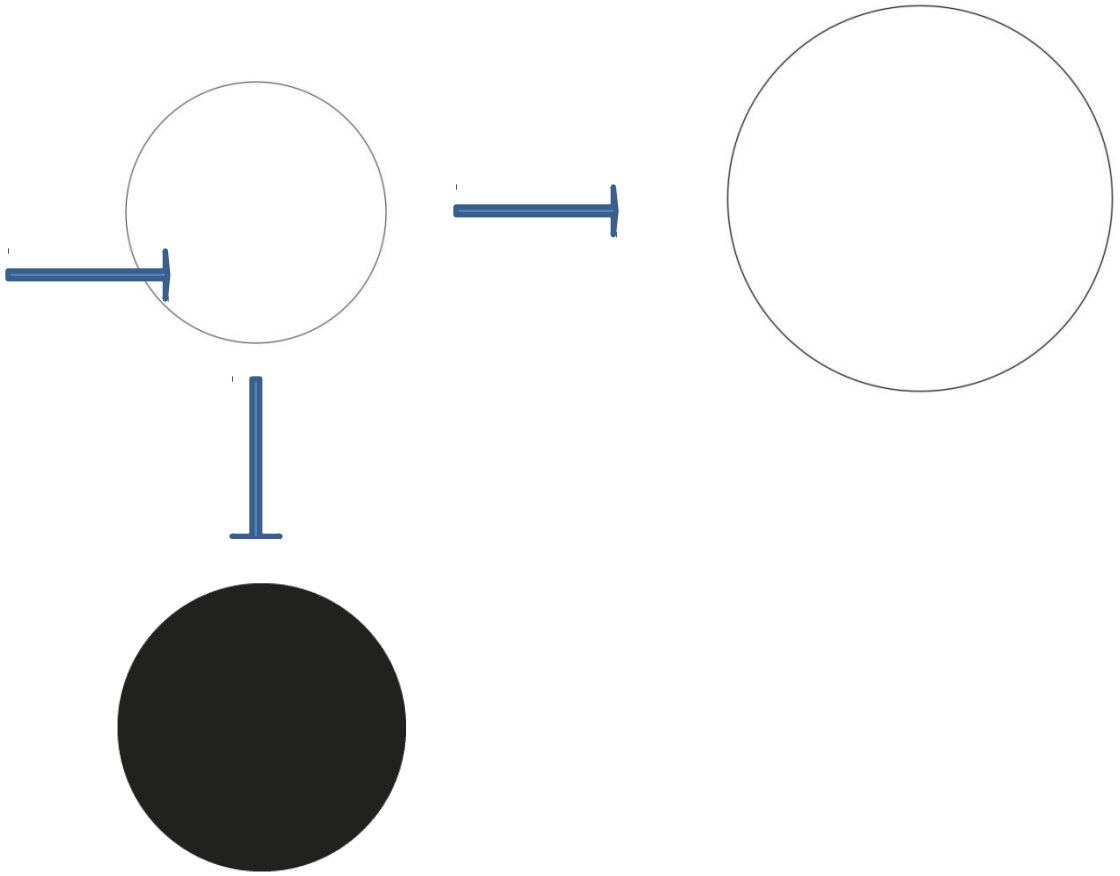




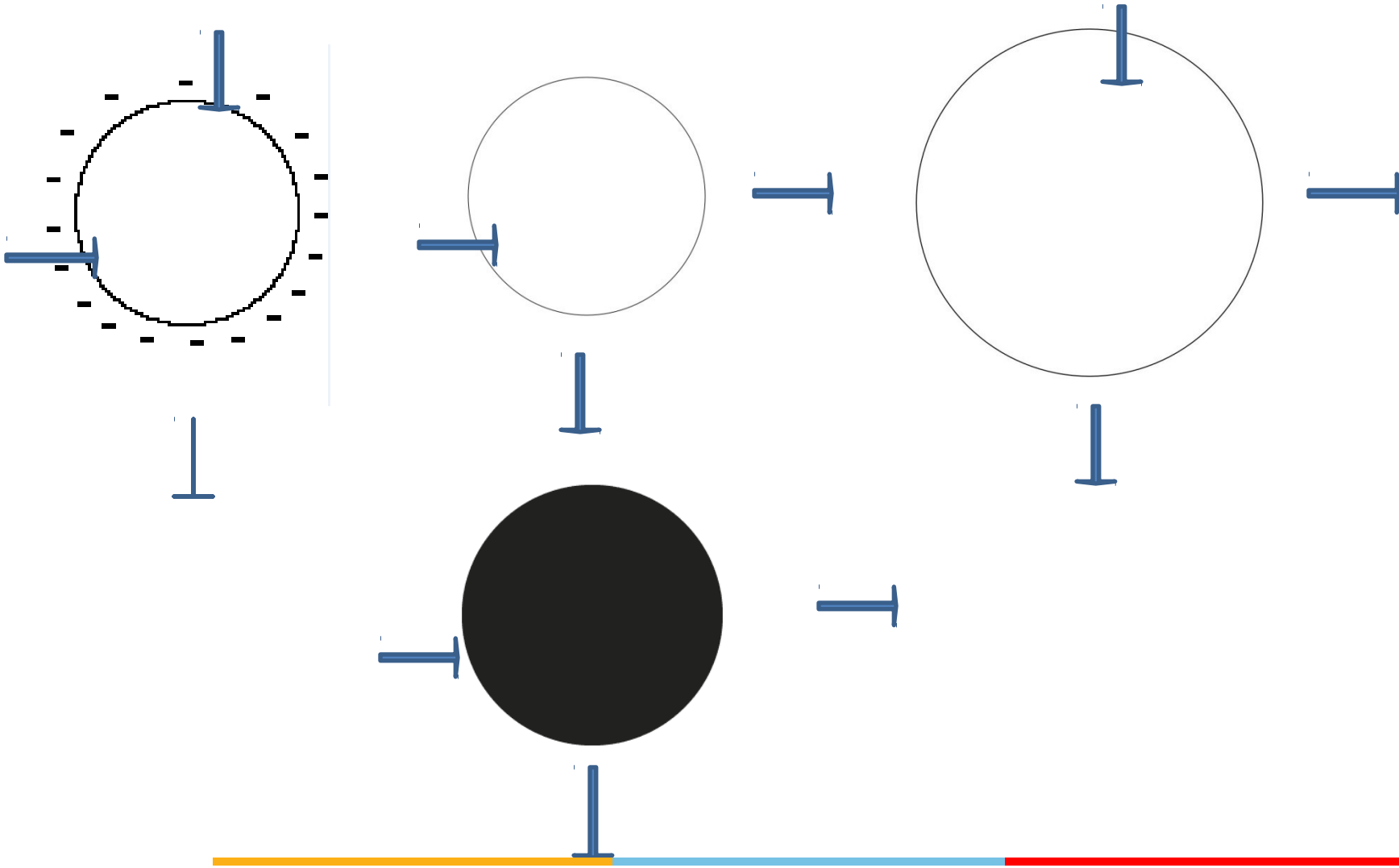
Type 0







More Than One Asymmetry



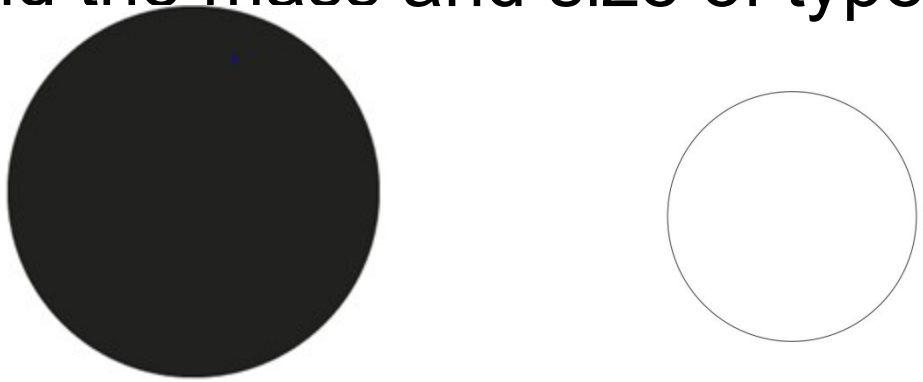
Mass and Size

Suppose we have a symmetric mixture of two particles:

Type 0 Type 1

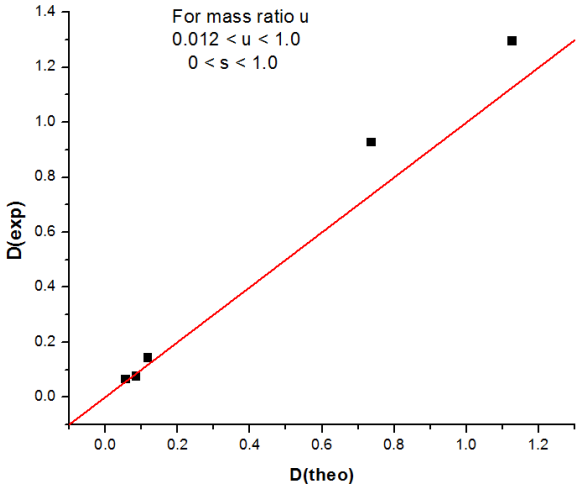
Now we introduce Mass as well as Size asymmetry in the mixture by increasing the mass and size of type 0 particle.

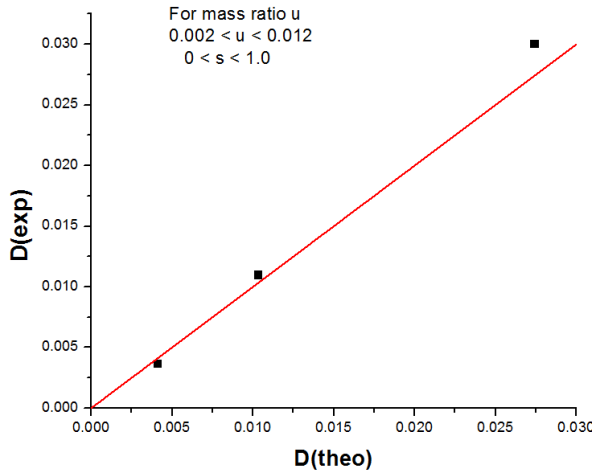
So the system looks lik



Analysis

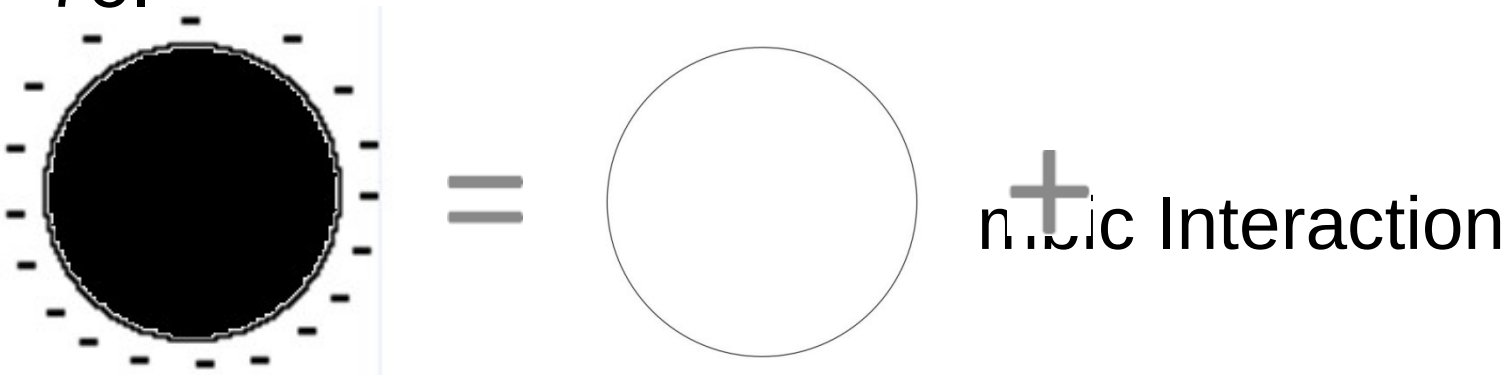
- We performed MD simulation for this new system with mass and size asymmetry.
- We express this diffusion coefficient (D) of this system in terms of mass asymmetry(μ), size asymmetry(s), diffusion coefficient of a system with only mass asymmetry (DM), diffusion coefficient of a system with only size asymmetry (DS).





Mass and Charge

- For a system with asymmetry in mass and charge MD simulation was carried out.
- Diffusion coefficient (D) for this charged system with or without asymmetry in mass was determined in terms of packing fraction (η) of neutral particle, packing fraction of charged particle, Diffusion Coefficient of neutral particle and charge of the particle, for a system with relative permittivity(Ɛr) 0f 78.



Results

Structural Properties

- Almost no change in equilibrium structure with mass asymmetry was observed.
- The system tends to move towards inhomogeneity with increase in size asymmetry.
- Charge separation takes place on increasing the charge asymmetry.

Transport Properties

- Diffusion Coefficient decreases with Increase in Mass Asymmetry.
- Diffusion Coefficient decreases with increase in Size Asymmetry.
- Diffusion Coefficient decreases with increase in Charge Asymmetry.
- Activation Energy for Diffusion Increases with increase in mass asymmetry.
- Collision frequency decreases with increase in mass asymmetry.